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(54) Title: ISOPENICILLIN N SYNTHETASE AND DEACETOXYCEPHALOSPORIN C SYNTHETASE ENZYMES AND METHOD

A three-dimensional structure is described of a complex of isopenicillin N synthase (IPNS) with Fe and its substrate ACV. This structure is used to design modified enzymes IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, which modified enzymes may accept unnatural substrates or improve production efficiency or produce improved products. Specific modifications of specific amino acid residues are proposed and exemplified.

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ISOPENICILLIN N SYNTHETASE AND DEACETOXYCEPHALOSPORIN C SYNTHETASE ENZYMES AND METHOD

5 Introduction

All commercially used penicillin and cephalosporin antibiotics and their derivatives are produced from fermentation derived materials containing a β -lactam ring. A range of organisms, including both prokaryotes and eukaryotes, and conditions may be used for their fermentation. Some are produced directly by fermentation followed by isolation. Others are produced by modification of materials produced by fermentation. Commercially used cephalosporins (also known as cephems) may be produced by modification of either fermentation derived penicillins or cephalosporins.

The biosynthetic pathway to the penicillins and cephalosporins has been extensively studied and involves the following steps (Scheme 1):

- 1. Three amino acids (<u>L</u>-α-aminoadipic acid, <u>L</u>-cysteine, <u>L</u>-valine) are condensed to form a tripeptide: <u>L</u>-δ-α-aminoadipoyl-<u>L</u>-cysteinyl-<u>D</u>-valine (ACV). During this process the <u>L</u>-valinyl residue is converted to a <u>D</u>-valinyl residue. This process is catalysed *in vivo* by the enzyme ACV synthetase and is common to both penicillin and cephalosporin biosynthesis.
- 2. ACV is converted to isopenicillin N in a step catalysed by the enzyme isopenicillin N synthase (IPNS). This step is common to both penicillin and cephalosporin biosynthesis.
 - 3. In some organisms (e.g. Penicillium chrysogenum and Aspergillus nidulans) isopenicillin N is converted by exchange of its \underline{L} - δ - α -aminoadipoyl side chain to penicillins with other side chains, which are normally more hydrophobic than the side chain of isopenicillin N. This

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conversion may be catalysed by an amidohydrolase/ acyltransferase enzyme. Examples of penicillins produced by this biosynthetic process include penicillin G (which has a phenylacetyl side chain) and penicillin V (which has a phenoxyacetyl side chain). These hydrophobic penicillins may be commercially produced by fermentation under the appropriate conditions.

- 4. In some organisms (e.g. Streptomyces clavuligerus and Cephalosporium acremonium) isopenicillin N is epimerised to penicillin N. This reaction is catalysed by an epimerase enzyme.
- 10 5. In some organisms (e.g. S. clavuligerus and C. acremonium) penicillin N is converted to deacetoxycephalosporin C (DAOC). This reaction is catalysed by deacetoxycephalosporin C synthase (DAOCS) in some organisms (e.g. Streptomyces clavuligerus) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others

 15 (e.g. C.acremonium).
 - 6. In some organisms (e.g. *S. clavuligerus* and *C. acremonium*) DAOC is converted to deacetylcephalosporin C (DAC). This reaction is catalysed by deacetylcephalosporin C synthase (DACS) in some organisms (e.g. *S. clavuligerus*) and by deacetoxy/deacetylcephalosporin C synthase (DAOC/DACS) in others (e.g. *C. acremonium*).

Further biosynthetic steps to give other cephalosporin derivatives may also occur, e.g. in *C. acremonium* DAC may be converted to cephalosporin C and in *Streptomyces spp*. DAC may be converted to cephamycin C. The genes encoding for each of the enzymes catalysing steps 1-6 above have been identified and sequenced.

Fermented penicillins, cephalosporins, their biosynthetic intermediates, and their derivatives may be of use as antibiotics or as intermediates in the production of antibiotics. Penicillins with hydrophobic side chains may be used for the preparation of cephalosporins or intermediates used in the preparation of cephalosporins, e.g. penicillins

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(including, but not exclusively, penicillin G and penicillin V) may be used to prepare C-3 exomethylene cephams which may be used as intermediates in the preparation of the commercial antibiotics, *e.g.* Cefachlor (Scheme 2).

For reviews see J. E. Baldwin and C. J. Schofield, in 'The Chemistry of β-lactams (Ed. M. I. Page), Chapter 1, Blackie, London 1992; Aharonowitz *et al*, Ann. Rev. Microbiol., 1992, <u>46</u>, 461; Cooper, Bioorg. Med. Chem., 1993, <u>1</u>, 1; Baldwin and Abraham, Nat. Prod. Report., 1989, <u>5</u>, 129; Baldwin, J. Heterocyclic. Chem., 1990, <u>27</u>, 91.

10 Summary of Invention

This invention is based on our determination of the three-dimensional structure of IPNS. That the structure of IPNS complexed to manganese has been determined, was reported by some of us in Nature, Volume 375, 22 June 1995, pages 700-704. That publication did not include the co-ordinates of the individual amino acid residues, and these are now provided. Scheme 2 of that paper contains the amino acid sequence of IPNS, and also DACS, DAOCS and DAOC/DACS and other structurally related enzymes, each of which is published in Swissprot or Genbank or other database.

We have now determined the structure of a complex of IPNS with Fe and ACV which is a substrate for the enzyme (see Scheme 1). In solution it is this complex, and not the IPNS-Mn complex, that is actually formed during step 2 of the biosynthesis of bicyclic β-lactams. Because the amino acid sequences of DAOCS, DAOC/DACS, DACS and other oxidases and oxygenases are so similar to that of IPNS, it is reasonable to expect that the structures of those enzymes are at least similar to that of IPNS.

We have also determined the structures of complexes of IPNS with Fe and with various analogues of ACV (in which another amino acid replaced <u>L</u>-valine), specifically AC glycine, AC aminobutyrate, AC

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alanine and AC proparglyglycine. These structures have been determined in the absence and in the presence of nitrous oxide NO. Exposure of these complexes to dioxygen alters the structures, and these altered structures have also been determined by us. From information given herein about the IPNS-Fe-ACV complex, a skilled reader is able to make and characterise the other complexes referred to in this paragraph, so structural details of those other complexes are not given herein.

Thus in one aspect the invention provides Isopenicillin N synthase (IPNS) in the form of: a complex with Mn having a structure designated by the X-ray co-ordinates in Table 2; or a complex with Fe and its substrate, said complex having a structure designated by the X-ray co-ordinates in Table 3.

In another aspect the invention provides Isopenicillin N synthase (IPNS) in the form of: a complex with Fe and an analogue of its substrate, either in the absence or in the presence of nitrous oxide or dioxygen, said complex having a structure designated by X-ray coordinates analogous to that set out in Table 3.

An analogue of an IPNS substrate is a substrate oxidised by IPNS to give preferably (but not exclusively) a bicyclic compound containing a β -lactam ring.

Table 2 sets out co-ordinates of individual amino acid residues in a crystalline complex of IPNS with manganese.

Table 3 sets out co-ordinates of individual amino acid residues in a crystalline complex of IPNS with Fe and ACV.

Knowledge, derived from the X-ray co-ordinates, of the three-dimensional structures of this family of related enzymes permits a skilled worker to identify specific amino acids that might be changed in order to alter or improve the properties of the enzyme in some way. While it is not possible from 3D structural information alone to predict that a specific amino acid mutation will produce a specific change in the properties of the

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enzyme, it is possible to identify a rather small number of amino acid residues where modification may be expected to change/improve the properties of the enzyme. The problem of identifying useful amino acid mutations is thus reduced to a level where it can readily be tackled by routine screening procedures.

Thus in one aspect the invention provides use of the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOCS/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for the modification of a second selected from IPNS, DAOCS, DACS, DAOCS/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway.

The three dimensional structure of a first enzyme may be the three dimensional structure of the IPNS-Fe-substrate complex referred to above. It may, however, also be that of DAOCS, DACS, DAOC/DACS or another oxygenase/oxidase related by sequence or structure (e.g. 1-aminocylopropane-1-carboxylic acid oxidase) to any of IPNS, DAOCS, DACS or DAOC/DACS. The structure of the IPNS-Fe-ACV complex may be derived from two or more crystalline polymorphs, all of which are envisaged. The structure may alternatively be of the enzyme in free form or in the form of some other complex such as with Mn, or with other Fe or ACV analogues, or enzyme inhibitors, or other enzyme modifiers. Preferably the second enzyme is the same as the first enzyme e.g. the 3D structure of IPNS is used as a basis for modifying IPNS. Alternatively the 3D structure of one first enzyme may be used as a basis for modifying a second structurally related enzyme.

Central to the elucidation of the structure of crystalline proteins is the discovery of conditions for the production of crystals with diffract X-rays to a sufficiently high resolution. Since the cofactors (e.g. Fe(II)) and substrates (e.g. ACV) of the family of enzymes to which IPNS, DAOCS, DACS, etc. belong are sensitive to modification by reaction with

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dioxygen, the crystallisation of these enzymes is preferably carried out under an anaerobic atmosphere or one containing only a very low concentration of dioxygen.

The modified enzyme(s) may be used in vitro or introduced via recombinant molecular biology techniques into an organism so that new materials can be fermented. It is recognised that multiple modifications may have to be made to an enzyme in order to change its substrate/product selectivity, and/or improve it efficiency. It is recognised that more than one modified enzyme may be used to effect the desired transformation. It is recognised that in order to change the nature of the enzyme-substrate/intermediate/product interactions at a particular enzymesubstrate/intermediate interface modifications may be made to the enzyme either immediately at the interface or away from it. It is recognised that the modifications may result in hybrid enzymes containing sequences from, e.g. IPNS and DAOCS or IPNS and DACS or any combination of IPNS, DAOCS, DACS or DAOCS/DACS or other related enzymes. It is also recognised that it may be desirable to further modify the organism in which the modified enzyme is to be introduced, e.g. by blocking a particular pathway in that organism (using the techniques of molecular biology) in order to modify flux through the desired/modified pathway, by introducing other enzyme activities, or by other modifications. The organism into which the modified enzyme will be used may or may not contain parts of the penicillin and cephalosporin biosynthetic machinery. The organism may already have been modified to optimise or minimise production of particular products or consumption of particular nutrients. More than one modified enzyme may be used in conjunction either in vitro or in vivo in an organism for the production of desirable products.

While modifications for numerous specific purposes are discussed below, it is possible to say in general that useful modifications will be of three kinds:

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- Those which permit the enzyme to accept unnatural substrates [i.e. substrates not normally present in the organism (which may or may not be an organism in which the enzyme is naturally occurring) in which the enzyme is operating] for the preparation of new or commercially valuable anti-bacterial materials or intermediates for the production of pharmaceutical products;
- Those which enable the enzyme to produce unnatural products [i.e. products not naturally produced in the organism in which the enzyme is operating, including 3-exomethylene cephams and cephalosporins with hydrophobic side chains at the C-7 position such as phenylacetamido or phenoxyacetamido, or other unnatural side chains such as adipoyl] or improve the production of natural products of commercial value.
- Those which enhance the ability of the enzyme to produce useful products. For example DAOCS is known to catalyse the production of phenylacetylcephalosporin C from penicillin G (Baldwin et al., Proceedings of the 7th International Symposium on the genetics of Industrial Micro-organisms, Abstract, p262, 1994). However, this conversion is much less efficient than the DAOCS catalysed conversion of penicillin N to DAOC. Modifications made to DAOCS may increase the efficiency of its catalytic conversion to penicillin G.

In another aspect this invention provides modified enzymes that result from application of the aforementioned techniques. These are enzymes having significant (as defined below) sequence and thus structural similarity with IPNS. Thus, structures of these enzymes may be predicted on the basis of the IPNS structures. Preferably there will be sequence similarity/identity between most of the modified enzyme and a major part of IPNS. Previous sequence comparisons (Roach *et al.*, Nature, 1995, 375, 700), using pairwise comparisons of the sequences followed by single linkage cluster analysis show that IPNS, DAOCS, DACS and

DAOC/DACS cluster with standard deviations scores of >5.0 (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Scores over 5.0 and preferably over 6.0 indicate that the sequence alignments will be correct within all or most of the protein secondary structural elements (Barton, Methods in Enzymol., 1990, 183, 403); thus they have significantly similar sequences and hence structures. Note there are other criteria which may be used to ascertain significant sequence similarity for example % identity or % similarity of amino acids possessing side chains with similar physicochemical properties (Barton and Sternberg, J. Mol. Biol., 1987, 198, 327). Thus, on the basis of sequence comparisons it is possible to predict the 10 structure of one enzyme (e.g. DAOCS, DACS or DAOC/DACS) from another (e.g. IPNS). Further, it is recognised that although two enzymes may have structures in which secondary structural elements are largely or wholly conserved, differences in the structures of the two enzymes may result from the side chains of the amino acids forming the secondary 15 structural elements. These differences, which may alter the substrate/product selectivities of the compared enzymes, may be predictable if the three dimensional structure of one of the enzymes is known. An example: the natural substrate for IPNS, ACV, has an Lconfigured aminoadipoyl side chain, whereas the substrates for DAOCS, 20 DACS and DAOC/DACS, i.e. penicillin N and DAOC, have D-configured aminoadipoyl side chains. This difference in selectivity may result from the different arrangement of amino acid side chain binding sites between IPNS and DAOCS, DACS, and DAOC/DACS, Further, it is recognised that there may be significant variations between enzymes which show significant 25 sequence/structural similarity (i.e. with standard deviation scores >5.0) in exterior regions of the enzymes, e.g. in loops and at the N- and C- termini. The relative importance of these regions in substrate binding may be predicted by comparison with a known crystal structure of an enzyme with significant sequence similarity. 30

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In one aspect, at least one of the following amino acid residues is modified:

R287; R87; R88; Y189; S183; Y91; F285; Q330; T331; V185; L106; C104; V217; L324; L317; I325; L321; S210.

The residue numbering herein is taken from the paper Nature, 1995, 375, 700-704 referred to above. These modifications are expected to have an effect on side chain substituents at the 6-position of the penicillin molecule, or the 7-position of the cephalosporin molecule. In each case, the stated amino acid residue may be replaced by the residue of any other amino acid. But in order to change the selectivity of the enzyme to accept substrates with hydrophilic or neutral side chains, the replacement is preferably to make the side chain binding pocket more hydrophobic.

In another aspect at least one of the following amino acid residues is modified:

V272; L231; L223; P283; T221; F211; F285; Q330; I187; V185; Y189; R279; S281; N230; Q225; N252; S210.

These modifications are expected to be associated with changes in the ring structure of the penicillin/cephalosporin molecule.

There follow examples of specific changes envisaged as a result of these modifications.

- a) The structure of IPNS is modified in its active site region to accept unnatural substrates to produce penicillins or other bicyclic β -lactams of commercial use with hydrophobic side chains (Scheme 5).
- The process may include the following modifications (other modifications based on the use of the crystal structure of IPNS are not excluded):

Note, R87F/A/G/V/L/I/T/W/M/C/N/Q/P/S/T/E/D/R/K/H indicates that residue arginine-87, using the *Aspergillus nidulans* IPNS numbering scheme is modified to phenylalanine or alanine etc. See Roach et al Nature, 1995, 375, 700-704.).

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R287F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/Y R87F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/Y Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y V185F/A/G/L/I/W/T/M/C/N/P/S/E/D/R/K/H/Q/Y L106F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y C104F/A/G/V/L/I/T/W/M/N/P/S/E/D/R/K/H/Q/Y V217F/A/G/L/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y L324F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y L317F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y 1325F/A/G/V/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y L321F/A/G/V/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

Note in these and in subsequently proposed modifications the
amino acid residue numbering scheme is based upon that used for
A. nidulans IPNS and the sequence alignments in Roach et al Nature,
1995, 375, 700-704, e.g. arginine-87 in IPNS remains named as arginine87 for other aligned enzymes.

It is recognised that modifications to the side chain binding
interactions and the valinyl binding interactions of IPNS may have to be
made in conjunction with each other or with other modifications in order to
produce a useful catalyst with the desired properties. Other modifications
based on the use of the three dimensional structures of IPNS, DACS,
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of
these enzymes to their substrates, intermediates, modifiers, products or

inhibitors are not excluded.

b) The structure of IPNS is modified in its active site region to accept natural or unnatural substrates to produce bicyclic β -lactams other than penicillins of commercial use (Scheme 6). For example the region of IPNS interacting with the valinyl residue of ACV may be modified such that IPNS produces 3-exomethylenecephams from ACV or other substrates for IPNS. The process may include the following modifications.

10	V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	P283F/A/G/V/I/LW/M/C/N/S/T/E/D/R/K/H/Q/Y
	T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
15	F211A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	F285A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	Q330F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
	I187F/A/G/LW/T/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	V185F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
20	Y189F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
	R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
	S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y
	N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
	Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
25	N252F/A/G/V/I/LW/M/C/P/S/T/E/D/R/K/H/Q/Y
	S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that modifications may have to be made in conjunction with each other or with other modifications to IPNS in order to produce a useful catalyst with the desired properties. Other modifications

based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

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The side chain binding interactions of IPNS are modified such that 6-aminopenicillins or other bicylic β -lactams may be produced *in vitro* or *in vivo* from dipeptides, such as cysteinyl-valine or other dipeptides (Scheme 7). Dipeptides may be produced (either *in vitro* or *in vivo*) by the use of a peptide synthetase enzyme, such as ACV synthetase (which may be modified by mutagenesis or other techniques to optimise dipeptide production) or by chemical synthesis. The process may include the following modifications:

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R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y
T331F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
C104F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V217F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

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d) The side chain binding interactions of IPNS are modified such that penams without any substituent at the 6-position or other bicylic β-lactams, without any substituent at the 6-position, may be produced *in vitro* or *in vivo* from dipeptides or amide substrates, such as 3-mercaptopropionyl-valine or other dipeptides or amides (Scheme 8). The dipeptides or amides may be produced (either in vitro or in vivo) by the use of a peptide synthetase enzyme, such as ACV synthetase (which may be modified by mutagenesis or other techniques to optimise dipeptide production) or by chemical synthesis. The process may include the following modifications:

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R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y T331F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L106F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y
V217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I325F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

- It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, products, modifiers, or inhibitors are not excluded.
 - e) IPNS is modified to produce 3-exomethylenecephams with hydrophobic or other unnatural side chains (Scheme 9) (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor. The process will involve modification of both the side chain binding interactions of IPNS substrates and of the valine binding interactions and may involve the use of ACV as a substrate or the use of other unnatural substrates. The process may include the following modifications, which may be made in conjunction with each other:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y Y189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R S183F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y

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Y91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y Q330F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y T331F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y V185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y L106F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y C104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y V217F/A/G/L/IW/M/C/N/P/S/T/E/D/R/K/H/Q/Y L324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y I325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y L321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y L231F/A/G/V/IW/M/C/N/P/S/T/E/D/R/K/H/Q/Y L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y P283F/A/G/V/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y F211A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y 1187F/A/G/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V V185F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y Y189F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y N230F/A/G/V/I/LW/M/C/P/S/T/E/D/R/K/H/Q/Y Q225F/A/G/V/I/LW/M/C/N/P/S/T/E/D/R/K/H/Y N252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y S210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y

It is recognised that these modifications may have to be
made in conjunction with each other or with other modifications in order to

produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded. The use of a modified IPNS in conjunction with another modified or unmodified oxygenase enzyme (e.g. DAOCS, DAOC/DACS) is not excluded.

f) The structure of DAOCS is modified in its active interactions region to accept substrates (*i.e.* penicillins with hydrophobic side chains, (including, but not exclusively, penicillin G and penicillin V) to produce cephalosporins or other bicyclic β-lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 10). The process may include the following modifications:

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R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M217F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V
1324F/A/G/V/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/L
1317F/A/G/V/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/L
Y321F/A/G/V/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y/L

R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be

made in conjunction with each other or with other modifications in order to
produce a useful catalyst with the desired properties. Other modifications
based on the use of the three dimensional structure of IPNS, DACS,
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of
these enzymes to their substrates, intermediates, modifiers, products or
inhibitors are not excluded.

g) The structure of DAOCS is modified in its active interactions region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, isopenicillin N, adipoyl penicillin) to produce bicyclic β-lactams other than cephalosporins of commercial use. For example the region of DAOCS interacting with the thiazolidine ring of its natural substrate penicillin N may be modified such that the modified DAOCS produces 3-exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS (Scheme 11). The process may include the following modifications:

V272F/A/G/I/LW/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/LW/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/LW/M/C/N/P/S/E/D/R/K/H/Q/Y
M211F/A/G/V/I/LW/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V
P185F/A/G/I/LW/M/C/N/S/T/E/D/R/K/H/Q/Y/V
F189A/G/V/I/LW/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V

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R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
F252F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be
made in conjunction with each other or with other modifications to DAOCS
in order to produce a useful catalyst with the desired properties. Other
modifications based on the use of the three dimensional structure of IPNS,
DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or
complexes of these enzymes to their substrates, intermediates, modifiers,
products or inhibitors are not excluded.

h) The side chain binding interactions of DAOCS are modified such that 6-aminopenicillins or other bicylic β -lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins, such as 6-aminopenicillanic acid (Scheme 12). The process may include the following modifications (other modifications based on the use of the three dimensional structures of IPNS or DAOCS or DAOCS/DACS are not excluded):

25 R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
30 F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y

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A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/V/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M217F/A/G/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I324F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
I317F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/I
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

i) The side chain binding interactions of DAOCS is modified such that cephams or cephalosporins without any substituent at the 7-position or other bicylic β-lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates (Scheme 13). The penicillanic acid may be produced whether in vitro or in vivo. The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y

C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y/
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/C/P/S/E/D/R/K/H/Q/Y
M217F/A/G/V/L/I/W/M/N/C/N/P/S/T/E/D/R/K/H/Q/Y
I324F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/I
Y321F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/I
R210F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/I

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It is recognised that the modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

j) DAOCS is modified to produce 3-exomethylenecephams with hydrophobic side chains (Scheme 14) (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cefachlor.) The process will involve modification of both the side chain binding interactions of DAOCS substrates and of the thiaxolidine binding interactions and may involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may include the following modifications (other modifications based on the use of

the three dimensional structures of IPNS or DAOCS or DAOCS/DACS are not excluded):

	V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
5	L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
	T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y
	M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F
10	L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V
	P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V
	F189A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
	S281F/A/G/V/I/L/W/M/C/N/P/T/E/D/R/K/H/Q/Y
15	N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
	Q225F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Y
	F252A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
	R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
20	R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
	C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
	T91F/A/G/V/L/I/W/M/C/N/Q/P/S/E/D/K/H/R/Y
	F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
	A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
25	P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
	T104F/A/G/V/L/I/W/M/N/P/S/T/E/D/R/K/H/Q/Y
	M217F/A/G/L/I/V/W/C/N/P/S/T/E/D/R/K/H/Q/Y
	1324F/A/G/L/V/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
	1317F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
30	R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I

PCT/GB97/02838

Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

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It is recognised that these modifications may have to be 5 made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or 10 inhibitors are not excluded.

The structure of DACS is modified in its active site region to k) accept substrates with hydrophobic side chains, including, but not exclusively, penicillin N, penicillin G and penicillin V) to produce cephalosporins or other bicyclic β -lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 15). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y 20 R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y 25 F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q P185F/A/G/L/IW/M/C/N/V/S/T/E/D/R/K/H/Q/Y T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y 30

R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

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It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

I) The structure of DACS is modified in its active site region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, adipoyl penicillin) to produce bicyclic β-lactams other than cephalosporins of commercial use (Scheme 16). For example the region of DAOCS interacting with the thiazolidine ring of its natural substrate penicillin N may be modified such that the modified DAOCS produces 3-exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS. The process may include the following modifications

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V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y/
M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F
L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V

P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V
R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y
S281F/A/G/V/I/L/W/M/N/C/N/P/T/E/D/R/K/H/Q/Y
N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y
Q225F/A/G/V/I/L/W/M/N/C/N/P/S/T/E/D/R/K/H/Y
F252F/A/G/V/I/L/W/M/N/C/P/S/T/E/D/R/K/H/Q/Y
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be
made in conjunction with each other or with other modifications in order to
produce a useful catalyst with the desired properties. Other modifications
based on the use of the three dimensional structure of IPNS, DACS,
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of
these enzymes to their substrates, intermediates, modifiers, products or
inhibitors are not excluded.

m) The side chain binding interactions of DACS are modified such that 7-aminocephems or 7-aminocephams (including 3-exomethylencephams) or other bicylic β -lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins (such as 6-aminopenicillanic acid) or cephams or cephems (Scheme 17). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/R/Y

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A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y,
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

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It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

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n) The side chain binding interactions of DACS are modified such that cephams or cephalosporins without any substituent at the 7-position or other bicylic β -lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates, such as penicillanic acid (Scheme 18). The penicillanic acid may be produced whether in vitro or in vivo. The process may include the following modifications:

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R287F/A/GN/L/IW/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/GN/L/IW/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/GN/L/IW/M/C/N/Q/P/S/T/E/D/K/H/Y
F189R/A/GN/L/IW/M/C/N/Q/P/S/T/E/D/K/H/Y
C183F/A/GN/L/IW/M/N/Q/P/T/E/D/K/H/R/Y/S

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S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/I
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

o) DACS is modified to produce 3-exomethylenecephams with hydrophobic side chains (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor.) (Scheme 19). The process will involve modification of both the side chain binding interactions of DACS substrates and of the thiaxolidine or cepham binding interactions and may involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may include the following modifications:

V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y

L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y M211A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y/F L187F/A/G/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/V 5 P185F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/V R279F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y S281F/A/G/V/I/L/W/M/N/C/N/P/T/E/D/R/K/H/Q/Y N230F/A/G/V/I/L/W/M/C/P/S/T/E/D/R/K/H/Q/Y Q225F/A/G/V/I/L/W/M/N/C/N/P/S/T/E/D/R/K/H/Y 10 F252F/A/G/V/I/L/W/M/N/C/P/S/T/E/D/R/K/H/Q/Y R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y F189R/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y 15 C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y A330F/GN/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y 20 T104F/A/G/V/L/I/W/M/N/P/S/E/D/R/K/H/Q/Y/C L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I Y321F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/L R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S 25

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS,

DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

p) The structure of DAOCS/DACS is modified in its active site region to accept natural or unnatural substrates (including, but not exclusively, penicillin N, adipoyl penicillin) to produce bicyclic β-lactams other than cephalosporins of commercial use (Scheme 20). For example the region of DAOCS/DACS interacting with the thiazolidine ring of its natural substrate penicillin N (or the cepham ring of DAOC) may be modified such that the modified DAOCS/DACS produces 3-exomethylenecephams from penicillin N, penicillin G, or penicillin V, or other substrates for DAOCS/DACS. The process may include the following modifications:

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V272F/A/G/I/LW/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P
T221F/A/G/V/I/LW/M/C/N/P/S/E/D/R/K/H/Q/Y/P
M211A/G/V/I/L/T/W/C/N/P/S/E/D/R/K/H/Q/Y/F
L187F/A/G/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V
P185F/A/G/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V
L189A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V
S281F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
S281F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
P1230F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y
R210F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y

R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

q) The side chain binding interactions of DAOCS/DACS are modified such that 7-aminocephems or 7-aminocephams (including 3-exomethylencephams) or other bicylic β-lactams may be produced *in vitro* or *in vivo* from 6-amino penicillins (e.g. 6-aminopenicillanic acid) or cephams or cephems (Scheme 21). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y
T217F/A/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y/I

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Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

r) The side chain binding interactions of DAOCS/DACS are modified such that cephams or cephalosporins without any substituent at the 7-position or other bicylic β -lactams, without any substituent at the 7-position, may be produced *in vitro* or *in vivo* from penicillins or cepham substrates, such as penicillanic acid. The penicillanic acid may be produced whether *in vitro* or *in vivo* (Scheme 22). The process may include the following modifications:

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R287F/A/GN/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/GN/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/GN/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R
C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S
S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y
F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y/
A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q
P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y
T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y

T217F/Å/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y
M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y
L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y
R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I
Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q
R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S
R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be
made in conjunction with each other or with other modifications in order to
produce a useful catalyst with the desired properties. Other modifications
based on the use of the three dimensional structure of IPNS, DACS,
DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of
these enzymes to their substrates, intermediates, modifiers, products or
inhibitors are not excluded.

exomethylenecephams with hydrophobic side chains (or other intermediates for use in the preparation of cephalosporin antibiotics, e.g. Cephachlor) (Scheme 23). The process will involve modification of both the side chain binding interactions of DAOCS/DACS substrates and of the thiaxolidine or cepham binding interactions and may involve the use of penicillins with hydrophobic side chains (e.g. penicillin G or V) as substrates or the use of other unnatural substrates. The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y
L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R

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S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I Y321F/A/G/V/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q V272F/A/G/I/L/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y L231F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y L223F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y V283F/A/G/I/L/W/M/C/N/S/T/E/D/R/K/H/Q/Y/P T221F/A/G/V/I/L/W/M/C/N/P/S/E/D/R/K/H/Q/Y M211A/G/V/I/L/T/W/C/N/P/S/E/D/R/K/H/Q/Y/F L187F/A/G/I/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y/V P185F/A/G/I/L/T/W/M/C/N/S/E/D/R/K/H/Q/Y/V F189A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Q/Y R279F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/K/H/Q/Y S281F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y N230F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y Q225F/A/G/V/I/L/T/W/M/C/N/P/S/E/D/R/K/H/Y F252F/A/G/V/I/L/T/W/M/C/P/S/E/D/R/K/H/Q/Y R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications

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produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS, DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

t) The structure of DAOC/DACS is modified in its active site region to accept substrates (i.e. penicillins with hydrophobic side chains, (including, but not exclusively, penicillin N, penicillin G and penicillin V) to produce cephalosporins or other bicyclic β -lactams of commercial use with hydrophobic or other unnatural side chains (Scheme 24). The process may include the following modifications:

R287F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y 15 R87F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y R88F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y L189F/A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/K/H/Y/R C183F/A/G/V/L/I/W/M/N/Q/P/T/E/D/K/H/R/Y/S S91F/A/G/V/L/I/W/M/C/N/Q/P/T/E/D/K/H/R/Y 20 F285A/G/V/L/I/W/M/C/N/Q/P/S/T/E/D/R/K/H/Y A330F/G/V/L/I/W/M/C/N/P/S/T/E/D/R/K/H/Y/Q P185F/A/G/L/I/W/M/C/N/V/S/T/E/D/R/K/H/Q/Y T104F/A/G/V/L/I/W/M/C/N/P/S/E/D/R/K/H/Q/Y T217F/A/G/L/I/V/W/M/C/N/P/S/E/D/R/K/H/Q/Y M324F/A/G/V/I/L/W/C/N/P/S/T/E/D/R/K/H/Q/Y 25 L317F/A/G/V/I/W/M/C/N/P/S/T/E/D/R/K/H/Q/Y R325F/A/G/V/L/W/M/C/N/P/S/T/E/D/K/H/Q/Y/I Y321F/A/G/V/I/LW/M/C/N/P/S/T/E/D/R/K/H/Q R210F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S 30 R190F/A/G/V/I/L/T/W/M/C/N/P/E/D/R/K/H/Q/Y/S

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It is recognised that these modifications may have to be made in conjunction with each other or with other modifications in order to produce a useful catalyst with the desired properties. Other modifications based on the use of the three dimensional structure of IPNS, DACS,

DAOCS, DAOCS/DACS, other sequence related enzymes or complexes of these enzymes to their substrates, intermediates, modifiers, products or inhibitors are not excluded.

Use can also be made of the 3D structure of IPNS to determine or predict the structure of other related enzymes which are not active in the penicillin or cephalosporin biosynthesis pathway. The structural information so obtained can then be used to modify the other enzyme or for designing an inhibitor for the other enzymes. Such other enzymes include flavone synthase, prolyl hydroxylase, proline hydroxylase, lysyl hydroxylase, aspartyl hydroxylase, flvanone 3β -hydroxylase, gibberellin C-20 oxidase, gibberellin 3β -hydroxylase, parahyroxyphenylpyruvate dioxygenase (HPPD), 1-aminocyclopropane-1-carboxylic acid (ACC) oxidase. Specific embodiments envisaged include:

- The modification of the oxidases involved in gibberellin biosynthesis in order that modified enzymes may be introduced into plants in order to improve crop production.
- The design of inhibitors of ACC oxidase to be used for the control of fruit ripening.
- The design and use of inhibitors of prolyl hydroxylase for use in the treatment of arthritis and related diseases.

Modification of enzymes may conveniently be effected at the nucleic acid stage. Thus, the present invention envisages genes which code for the modified enzymes herein described. The nucleic acid sequence of such genes may be readily predicted. Mutations of existing wild-type genes may readily be effected e.g. by the use of commercially available mutagenesis kits.

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The gene may be introduced into an expression vector by techniques which are well known. The expression vector may be used to transform a host micro-organism, such as for example Penicillium chrysogenum or Acremonium chrysogenum, again by techniques which are well known. The micro-organism should be capable of expressing the gene under fermentation conditions, e.g. by having the gene under the transcriptional and translational regulation of fungal expression signals. Such micro-organisms containing the modified gene may be used to make bicyclic β -lactams of the penicillin or cephalosporin family, again by techniques which are well known.

The following experiments were performed to demonstrate the invention.

EXAMPLE 1

A U.S.E mutagenesis kit (Phamacia) was used for all the mutagenesis reactions and a Pst I restriction site on the pET vector was selected. Selection of single and double mutants were successfully performed from colonies by restriction enzyme digestion. (Sambrook *et al*, Molecular Cloning, A Laboratory Manual, Cold Spring Harbour, USA, 1989). It was found that about 50% of colonies selected were mutants. Mutations of DAOCS (Table 1) were confirmed by sequencing according to the dideoxy method of Sanger. Mutants were designed after study of the IPNS-Mn²+ and the IPNS-Fe(II)-ACV structures. Polar residues with which the side chain D-α-aminoadipoyl (carboxylate and amino groups) might bind to were identified.

Almost all the mutants expressed well, except R88I, R88Q and R87Q/R287Q whereby the expression level was only about half of others. Generally the expression level of colonies was about 10~20 % of soluble protein at 27°C. Moreover, recombinant enzyme of P168V mutant was insoluble. These mutant enzymes were purified to ~60-70 % purity

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with Resouce-Q column (Phamacia). The activity of each mutant with respect to penicillin N and its side-chain analogues was analysed by bioassay. It was found that R87I, R87Q, R88I and R88Q could inhibit the growth of E coli X580 cells using a hole-plate assay which contained penicillinase. The products of the reaction with penicillin G and wild type DAOCS also showed the same inhibition. Screening of the substrate conversion of penicillins mutants was also performed using a assay with radiolabelled α -ketoglutarate. The reaction conditions were the same as for bioassay except that $[^{14}C]$ - α -ketoglutarate was used. The specific activities of the various mutants are summarised in Table I.

The loss of activity when using penicillin N as a substrate after mutation of arginine 287 to isoleucine or glutamine in the active site of expandase implies an important interaction of this amino acid with the carboxyl group which located in the side chain of penicillin N. This is compatible with the structural predictions for DAOCS which were suggested based on IPNS structure. On the other hand, mutation at arginine 87 to isoleucine or glutamine enhanced the activity (when using penicillin N as a substrate), whereas mutants of arginine 88 caused partial loss of activity (when using penicillin N as a substrate). Double mutations at the sites totally eliminated activity.

The specific activities of the (mutant) modified DAOCS, when using penicillin N as a substrate, support the prediction that the 3-dimensional structure of DAOCS is closely related to that of IPNS. However, not all the kinetic results can be predicted by analysis of the predicted DAOC structure, e.g. the apparent increase in activity of the R87Q modification, when using penicillin N as a substrate. Other results in Table 1 further demonstrate the invention. For example the R87Q mutant converts penicillin G to phenylacetylcephalosporin G more efficiently than the unmodified enzyme. Other results demonstrate the introduction of new activities into the modified DAOCS enzymes. For example neither oxacillin

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nor piperacillin are substrates for the unmodified enzymes, but are substrates for the R87I/R287Q modified enzymes.

EXAMPLE 2

IPNS-Fe-ACV Complex

Enzyme and Substrate Preparation

Recombinant *A. nidulans* IPNS was purified as the apoenzyme as described previously (Roach *et al*, Protein Science, 1995, **4**, 1007-1009) and stored at -80°C in 75 μ l aliquots (50 mg/ml in 20 mM Tris-HCl, pH 8.0). ACV (thiol form) was prepared as described previously and was further purified by HPLC [Hypersil octadecylsilane (C₁₈) column (250 x 10 mm), eluting with 10 mM NH₄CO₃, containing 4% (vol./vol.) MeOH; R_t=6.5 min at 4 ml/min], freeze dried and stored as 2 mg aliquots.

15 Crystallisation

Crystallisation trials were performed at 17°C under anaerobic conditions (<0.2 ppm O₂) in a glove box (Belle Technology, Portesham, Dorset, UK) using the hanging drop vapour diffusion technique. All solutions except the protein were deoxygenated by repeated evacuation followed by argon flushing (repeated three times) prior to transfer to the anaerobic glove box. Solid reagents (ACV, ferrous sulphate and sodium dithionite), all solutions except protein solutions, washed cover-slips and greased Linbro plates were left for 16 h in the glove box to further deoxygenate. IPNS solutions were transferred to the glove box immediately prior to each crystallisation experiment and mixed by repeated gentle pipetting to assist deoxygenation. To further ensure that the crystallisation experiments were done anaerobically, a coloured redox indicator was added to each well. Thus, oxidised resazurin which shows a mauve to colourless change upon dithionate reduction, was added (0.001% mass/vol.) to the stock well solutions (separate solutions, without

resazurin, were reserved for hanging drops) and sodium dithionite solution (100 mM) added dropwise until the solution in the well changed colour from mauve to colourless (Jacob, Methods in Microbiol., 1969, **2**, 91-124). Upon exposure to oxygen (either by contamination or upon withdrawing the crystallisation tray from the glove box), the solution in the well changed from colourless (reduced) to pink (partially oxidised).

A stock solution containing ferrous sulphate (5 mM), ACV (80 mM) and IPNS (50 mg/ml. 1.35 mM) was then prepared and used in random screening experiments using 6 µl drops (1:1 precipitant:protein) (Jancerik and Kim, J. Appl. Crystallog., 1991, **24**, 409). Three crystal forms were obtained using a precipitant solution containing 1.8M lithium sulphate and 100 mM Tris-HCI (pH 8.5). Crystals were not observed in analogous crystallisation experiments carried out in the absence of ACV. Crystallisation conditions were optimised by varying the protein and precipitant concentrations.

Plate crystals (Form I) typically appeared between 6 and 12 hours and reached a maximum size (typically 500 x 150 x 25 μ m³) in 48 hours. Hexagonal columnar crystals (Form II) typically appeared after 12 - 16 hours and grew to a maximum size (typically 1000 x 500 x 500 μ m³) in 1 week. The needles (Form III), with a hexagonal cross-section, appeared after *ca*. 2 weeks and were more commonly observed when using less homogenous batches of protein. In analogous experiments carried out under aerobic conditions, no crystals were observed.

Form I crystals grew spontaneously in less than half of the drops after 12 hours. After this time, Form II crystals began to grow and predominated in those drops in which plates had not grown. By using serial dilutions of microseeds prepared from either Form I or Form II crystals, it was possible to bias the growth of crystals completely to either of these morphologies. There is a delicate balance between production of the different forms since some drops contained two or all three of the

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different crystal forms.

X-ray Analysis

For initial characterisation, crystals were mounted in quartz capillaries under an anaerobic atmosphere and the capillaries sealed with wax. Data were then collected (Table 4) at room temperature. Subsequently, the crystals were shown to be apparently stable to relatively short (< 1 hour) exposure to oxygen and were withdrawn from the glove box. The crystals were then rapidly transferred to a cryoprotective mother liquor (100 mM Tris-HCl pH 8.5, 20% (vol./vol.) glycerol, saturated at room temperature with lithium sulphate) and frozen using a Cryostream (Oxford Cryosystems). Data were then collected at 100 K. Data were analysed using the programs DENZO and SCALEPACK (Otinowski, Data Collection and Processing, Daresbury Laboratory, Warrington, UK (Sawyer et al, Eds) PL/SCI/R34, pp 55-62). 15

Table 4 - Crystal Statistics

Crysta 1 Form	Diffractio n Limit (nm)†	Space Group	Unit Cell Dimensions (nm)	Solvent Content (%)	Completeness (%)	Rsym (%)
	0.11, 0.18	P2 ₁ 2 ₁ 2 ₁	4.68, 7.15, 10.10	38.5	95.4	5.9
11	0.21, 0.23	P3 ₁ 2 ₁	10.10, 10.10, 11.567	69.5	94.0	7.2

† The first figure refers to the diffraction limit of the form I and form II crystals after respectively 30 and 10s exposures at BL19 of the European 20 Synchrotron Radiation Facility (ESRF). The second figure refers to the diffraction limits after 30 min. exposures using a Rikagu rotating anode source operating at 60 kV and 70 mA equipped with a MAR Research

imaging plate detector. All other figures in the table refer to data collected at the ESRF. The data for form I crystals was collected using a MAR Research imaging plate detector and the data for the form II crystals on a charged coupled device detector.

Hereafter:

Table 1 appears on page 41.

Table 2 appears on pages 42-78.

Table 3 appears on pages 79-119.

Reaction Schemes on pages 120-129.

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Table 1: The Specific activity of various DAOCS mutants analysed by the turnover of lpha-[' 4 C]-ketoglutarate.

		6-Amino-									-		
Specific activity		penicillanic acid	Adipyl-6-	Penicillin G	penicillin V	Ampicillin	Carbenicillin	Ammoxicillin	Methicillin	Cloxacillin	Oxacillin	Piperacillin	
(nmol/min/mg)	Penicillin N	(6-APA)						4 440 6	0	1.6±0.6	0	0	
		10+0.2	2.7±0.4	5.1±0.4	5.3±0.3	0	0	4 4 10 04	0.2+0.1	2.7±0.6	2.0±0.09	1.8±0.2	
Wild type	6.4±0.5	17+06	0	0	2.3±0.2	0	0	to:0H .	0	0	0	0	, ,
R2871	> \		0	0	0	0	0 0		0	0.9±0.04	0.8±0.3	0	
R287Q	0 017	11+0.5	0	4.3±0.1	1.5±0.3	0	- C	,	0	0	0	0	
R871	0.4±0.05	0	0	7.5±0.4	3.4±0.6	0	>	,	0	0	0	0	
R87Q	13.410.4	,	0	2.5±0.5	0	0	>	,	0	0	0	0	
R88I	5.3±0.8	1	0	0.2±0.02	0	0	0	5 6	- c	0	0	0	ι
R88Q	2.9±0.5	_	, -	00.3±0.04	0	0	0	> \rightarrow{\circ}{\circ}	,	0	0	0	1
R871/R2871	0	→ \	,	0	0	0	0	0	, _c	4 5+0.08	4 1±0 4	2.5±0.3	Т
R870/R2871	0	0	,	3.2±0.1	0.7±0.2	0	0	1.1±0.3			0	0	Τ
R871/R2870	0	3.3±0.2		0	0	0	0	0	> 	_			7
R870/R2870	0	> \	,										

 * Experiments were done in duplicate and values for "the penicillin uncoupled decarboxylation of α -ketoglutarate" have been subtracted.

The specific radioactivity of the $\alpha\text{-ketoglutarate}$ used was ca. 0.057 $\mu\text{Ci}/\mu\text{mol}.$

N.B. "The penicillin uncoupled decarboxylation reaction" is the enzymatic turnover of α -ketoglutarate in the absence of penicillin substrate.



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							- 42 -				
CRYST1		59.200	127.000	120		Ta	ble 2				
SCALE1				0.000		90.00		00.00			
SCALE2				0.000		.00000			0.0000	0	
SCALE3				0.007		.00000			0.0000		
ATOM			B VAL	0.000		.00716	3		0.0000		
ATOM						6.524	53.636	ś .	-2.826		
ATOM		_				5.692	54.759		-2.223	1.00	
ATOM					4 18	3.011	53.869		-2.523	1.00	
ATOM		_	VAL		4 14	1.636	52.001		2.797	1.00	77.94
ATOM			VAL		4 14	.443	51.769			1.00	78.66
ATOM		6 N	VAL	A	4 16	.880	51.117		3.987	1.00	79.44
ATOM		7 C	A VAL	A	4 16	.049	52.254		2.818	1.00	82.21
ATOM		8 N	SER	A		.655	52.015		2.290	1.00	80.32
		9 CA			_	. 286	51.764		1.916	1.00	76.44
ATOM	1		SER .	A	_	.583			2.350	1.00	73.85
ATOM	1.		SER .	A		.012	50.804		1.380	1.00	74.99
ATOM	12	_	SER		_	.474	51.018		0.044	1.00	76.77
ATOM	13	3 0	SER A			.970	53.054	- :	2.482	1.00	70.80
ATOM	-14	N	LYS A		_		54.146	- 2	2.187	1.00	70.77
ATOM	15	CA				.250 .	52.914	- 2	2.970	1.00	
ATOM	16		LYS A			.320	54.025		3.124	1.00	67.33
ATOM	17		LYS A			403	53.799		.319	1.00	64.23
ATOM	18		LYS A			751	54.568		.557	1.00	65.78
ATOM	19					579	54.445		.510		69.46
ATOM	20		LYS A			768	55.261		. 784	1.00	76.71
ATOM	21	NZ	LYS A			509	55.312		.612	1.00	81.89
ATOM		C	LYS A		68.	457	54.095			1.00	83.94
ATOM	22	0	LYS A		_	061	53.061		.868	1.00	61.05
ATOM	23	N	ALA A		_	166	55.304		.325	1.00	62.18
ATOM	24	CA	ALA A		_	346	55.487		.410	1.00	55.41
ATOM	25	CB	ALA A	-	_	532	56.853		.231	1.00	49.08
	26	C	ALA A	7		375	56.853		. 393	1.00	44.79
ATOM	27	0	ALA A	7			55.363		609	1.00	46.39
ATOM	28	N	ASN A	8			55.706		721	1.00	44.68
ATOM	29	CA	ASN A	8			54.840	0.	313	1.00	45.74
ATOM	30	CB	ASN A	8			54.694	0.	086	1.00	
ATOM	31	CG	ASN A				53.759		142	1.00	46.86
ATOM	32	OD1	ASN A	8			53.798		154	1.00	53.92
ATOM	33	ND2	ASN A	8	•		53.318		226	1.00	59.91
ATOM	34	C		8			54.403		193		63.71
ATOM	35	0	ASN A	8	3.0		56.078		175	1.00	61.02
ATOM	36		ASN A	8	2.7	82	56.594		276	1.00	45.51
ATOM	37	И	VAL A	9	2.8	02	56.712	-0.9		1.00	49.10
ATOM		CA	VAL A	9	2.16	57	58.028			1.00	42.13
ATOM	38	CB	VAL A	9	3.06	6	59.093	-1.(1.00	36.18
ATOM	39	CG1	VAL A	9	2.42		60.459	-1.7		1.00	31.81
ATOM	40	CG2	VAL A	9	4.43		59.149	-1.6		1.00	28.09
ATOM	41	C	VAL A	9	0.83			-1.1		1.00	26.59
	42	0	VAL A	9	0.78		57.869	-1.7		1.00	36.23
ATOM	43	N	PRO A	10	-0.26		57.827	-3.0		1.00	39.84
ATOM	44	CD	PRO A	10	-0.32		57.715	-1.0		1.00	35.13
ATOM	45	CA	PRO A	10		_	57.622	0.4	51	1.00	33.70
ATOM	46	CB	PRO A	10	-1.58		57.549	-1.6	20	1.00	
ATOM	47	CG	PRO A		-2.47	_	57.229	-0.4	12	1.00	34.32
ATOM	48	C	PRO A	10	-1.77		57.912	0.7		1.00	35.22
ATOM	49	ō	PRO A	10	-2.09		58.759	-2.39	90	1.00	34.45
ATOM	50	N	LYS A	10	-1.77		59.897	-2.06	50	1.00	33.02
ATOM	51	CA	LYS A	11	-2.87		58.503	-3.43	34	1.00	36.04
ATOM	52	CB		11	-3.439		59.576	-4.23			35.45
ATOM	53		LYS A	11	-3.361		59.233	-5.72	o a	1.00	36.88
ATOM	54	CG	LYS A	11	-1.958		8.944	-6.20		1.00	31.82
ATOM	55	CD	LYS A	11	-1.858		8.929	-7.72	, ,	1.00	38.51
ATOM		CE	LYS A	11	-0.482		8.455			1.00	44.67
ATOM	56	NZ .	LYS A	11	0.620		9.309	-8.16	•	1.00	47.02
ATOM	57	С	LYS A	11	-4.882		9.740	-7.62		1.00	53.83
	58	0	LYS A	11	-5.748	_		-3.79		1.00	39.16
ATOM	59	N	ILE A	12	-5.133		8.984	-4.23		1.00	46.42
ATOM	60	CA	ILE A	12	-6.474		0.704	-2.91	7	1.00	36.94
ATOM	61		ILE A	12	-6.407		0.959	-2.39	4	1.00	32.90
ATOM	62		ILE A	12			1.510	-0.96	-	1.00	25.23
ATOM	63		ILE A		-7.803		1.826	-0.43	_	1.00	19.49
ATOM	64				-5.682	6	0.505	-0.07	7 :	1.00	
ATOM	65				-5.414		0.995	1.314		1.00	26.81
AŢOM	66				-7.268		1.932	-3.250	_	1.00	29.30
ATOM	67				-6.729		2.919	-3.749			38.45
ATOM	68				-8.544		1.622	-3.451		1.00	41.39
ATOM	69			13	-9.431		.484	-4.225		1.00	44.53
	• •	CD A	ASP A	13 -:	10.555		684	-4.881		1.00	46.03
								001	. 1	.00	51.16

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						5 060	1.00	56.62
	70	CG AS	SPA 1	3 -11.361	62.512	-5.869 -5.544	1.00	54.34
MOTA	70 71		SP A 1	3 -11.737	63.659		1.00	66.60
MOTA	72		SPA 1	3 -11.619	62.011	-6.984 -3.227	1.00	44.39
ATOM	73		SP A 1	3 -10.000	63.472	-2.354	1.00	44.73
ATOM		-		3 -10.791	63.121		1.00	44.33
ATOM	74	-		4 -9.605	64.719	-3.391	1.00	38.69
MOTA	75 76	-		4 -10.003	65.785	-2.498	1.00	34.66
ATOM	76			4 -8.796	66.720	-2.338	1.00	37.77
MOTA	77 78			4 -9.190	68.101	-1.875 -1.365	1.00	33.42
ATOM	75 79			4 -7.833	66.077	-2.846	1.00	39.30
ATOM	80			4 -11.296	66.521	-2.848	1.00	39.59
ATOM	81	-		L4 -11.808	67.298	-3.990	1.00	38.33
MOTA	82	_		15 -11.891	66.202	-4.393	1.00	37.64
MOTA				15 -13.116	66.881	-5.689	1.00	39.61
MOTA	83 84			15 -13.686	66.298	-5.546	1.00	47.59
ATOM	85			15 -14.027		-3.324	1.00	37.35
ATOM	86			15 -14.197			1.00	40.20
ATOM	87			15 -14.691		-3.056 -2.647	1.00	38.58
MOTA	88			16 -14.532	65.866	-2.714	1.00	40.22
ATOM	89		PRO A	16 -13.957	64.511	-1.613	1.00	37.63
MOTA	90	CA	PRO A	16 -15.574		-0.901	1.00	33.25
ATOM	91	CB	PRO A	16 -15.410		-1.991	1.00	36.58
MOTA		CG	PRO A	16 -14.999		-0.624	1.00	38.86
MOTA	92	C	PRO A	16 -15.43	9 67.066		1.00	40.71
MOTA	93 94	0	PRO A	16 -16.44		-0.184 -0.310	1.00	39.30
MOTA	95	N	LEU A	17 -14.20	0 67.444	0.649	1.00	38.18
MOTA	96	CA	LEU A	17 -13.91	7 68.513	0.911	1.00	34.24
ATOM	90 97	CB	LEU A	17 -12.41	2 68.594	1.490	1.00	32.70
ATOM	98	CG	LEU A	17 -11.83		1.663	1.00	27.81
MOTA		CD1	LEU A	17 -10.33	0 67.382	2.820	1.00	34.84
MOTA	99	CD2	LEU A	17 -12.51	.5 67.008		1.00	41.67
MOTA	100	C	LEU A	17 -14.47	69.881	0.260	1.00	38.36
MOTA	101	0	LEU A	17 -14.59		1.105	1.00	48.11
ATOM	102	N	PHE A	18 -14.77		-1.025	1.00	52.21
ATOM	103	CA	PHE A	18 -15.33	39 71.287	-1.551	1.00	51.38
MOTA	104	CB	PHE A	19 -14.8	57 71.551	-2.993	1.00	49.52
MOTA	105	CG	PHE A	18 -13.3	65 71.738	-3.132	1.00	50.16
MOTA	106	CD1	PHE A	18 -12.5	52 70.679	-3.513	1.00	47.59
MOTA	107	CD2	PHE A	18 -12.7	81 72.983	-2.932	1.00	50.47
ATOM	108	CE1	PHE A	18 -11.1	83 70.857	-3.695	1.00	44.37
ATOM .	109	CE2	PHE A	18 -11.4	13 73.166	-3.114	1.00	45.21
MOTA	110	CZ	PHE A	18 -10.6	16 72.102	-3.496 -1.550	1.00	53.42
MOTA	111	C	PHE A	18 -16.8	71 71.202	-1.848	1.00	53.80
MOTA	112	0	PHE A	18 -17.5		-1.259	1.00	56.82
ATOM	113	N	GLY A	19 -17.4			1.00	60.49
MOTA	114	CA	GLY A	19 -18.8		-1.247 0.120	1.00	64.67
MOTA	115	C	GLY A	19 -19.5		1.071	1.00	64.98
MOTA	116	0	GLY A	19 -18.	927 70.470		1.00	69.36
MOTA	117		ASP A	20 -20.	738 69.441	0.200 1.449	1.00	72.36
MOTA	118		ASP A	20 -21.	507 69.443		1.00	76.50
MOTA	119		ASP A	20 -22.	799 70.263	1.310	1.00	83.77
MOTA	120		ASP A	20 -22.	543 71.760	1.234	1.00	89.42
MOTA	121		ASP A	20 -21.	889 72.300	2.152	1.00	85.64
MOTA	122		ASP A	20 -23.	002 72.400	0.262	1.00	70.68
ATOM	123		ASP A	20 -21.	861 68.035	1.918	1.00	71.00
MOTA	124	_	ASP A	20 -22.	433 67.865		1.00	68.45
MOTA	129	-	ASP A	21 -21	.533 67.030		1.00	66.91
MOTA	126		ASP A	21 -21	.830 65.653		1.00	69.88
MOTA	12		ASP A	0.1	.643 64.720		1.00	73.83
MOTA	12		ASP A		.015 63.268		1.00	76.66
MOTA	1.2				.477 62.978		1.00	76.24
MOTA	13			01	.845 62.409	-0.322		65.51
MOTA	13	_	ASP A		.917 65.24	2.625	1.00	67.20
ATOM	13	_					1.00	63.04
ATOM	13		ASP A			5 3.838	1.00	00
MOTA	1.3		GLN A	20		8 5.033	1.00	00
MOTA	13					8 6.264	1.00	
MOTA	13	36 CB				0 7.505	1.00	
ATOM	13	37 CG		/		4 7.326		
ATOM	1	38 CE				6.649		0
ATOM	1	39 OE		1	J. U.J.			
MOTA	1	40 NE	E2 GLN		0.752		1.00	
MOTA	1	41 C	GLN		•		1.00	59.37
MOTA	1	42 0	GLN	A 22 -1	5.24-			

						- 44 -			
ATOM	1	43 N	ALA	λ.	2.2				
ATOM		44 C.			23 -20.8		4.428	1 00	
ATOM		45 CI			23 -20.44		4.323	1.00	
ATOM					23 -21.55	50 60.444	3.688	1.00	905
ATOM		_	ALA		23 -19.14	61.133		1.00	
ATOM		47 0	ALA		23 -18.18		3.547	1.00	58.62
		18 N	ALA	A	24 -19.11		4.040	1.00	59.15
ATOM	14	19 C			24 -17.92		2.329	1.00	57.88
ATOM	15	O CE		Δ		_ 01.50/	1.505	1.00	54.77
ATOM	15	1 C	ALA				0.097	1.00	
ATOM	15		ALA	•	24 -16.77		2.176	1.00	52.07
ATOM	15	_			24 -15.61		2.114		52.15
ATOM	15		LYS A		25 -17.09	7 63.443	2.835	1.00	55.14
ATOM	15				25 -16.08	7 64.230		1.00	46.23
ATOM					25 -16.690	65.505	3.516	1.00	42.19
ATOM	15		LYS A	Į.	25 -16.655		4.112	1.00	38.59
	15		LYS A	A	25 -17.022		3.149	1.00	33.56
ATOM	15	8 CE	LYS A		25 -18.525		3.806	1.00	35.11
ATOM	159	9 NZ	LYS A				3.890	1.00	
ATOM	160		LYS A		0		4.275	1.00	37.82
ATOM	161	_			25 -15.406		4.593		39.00
ATOM	162		LYS A		25 -14.186	63.378	4.688	1.00	43.50
ATOM			MET A		26 -16. 18 9	62.680		1.00	45.05
ATOM	163		MET A	2	26 -15.599		5.368	1.00	46.05
	164		MET A	2	26 -16.674	-2.0.2	6.424	1.00	51.52
ATOM	165		MET A	2	26 -17.065	61.263	7.306	1.00	58.77
ATOM	166	SD	MET A			62.138	8.503	1.00	
ATOM	167		MET A			62.302	9.788	1.00	68.62
ATOM	168	C			-15.385	60.571	10.146	1.00	75.98
ATOM	169	ō	MET A		6 -14.740	60.785	5.816		72.86
ATOM	170		MET A	2	6 -13.709	60.391	6.395	1.00	49.91
ATOM		N	ARG A	2	7 -15.148	60.307		1.00	49.46
ATOM	171	CA	ARG A	2	7 -14.407	59.273	4.645	1.00	50.27
	172	CB	ARG A	2			3.942	1.00	51.72
ATOM	173	CG	ARG A	2		58.858	2.662	1.00	59.72
ATOM	174	CD	ARG A	2	019	57.511	2.736	1.00	70.60
ATOM	175	NE	ARG A			57.084	1.365	1.00	
ATOM	176	CZ	ARG A	21		57.450	1.123	1.00	80.78
ATOM	177	NH1		27		58.133	0.056		88.62
ATOM	178		ARG A	27	7 -17.243	58.547	-0.867	1.00	93.71
ATOM		NH2	ARG A	27	-19.414	58.338		1.00	96.83
ATOM	179	C	ARG A	27		59.802	-0.135	1.00	97.09
ATOM	180	0	ARG A	27			3.585	1.00	48.21
	181	N	VAL A	28		59.115	3.794	1.00	49.76
ATOM	182	CA	VAL A	28		61.018	3.040	1.00	44.43
ATOM	183	CB	VAL A			61.637	2.669	1.00	
ATOM	184	CG1	VAL A	28		63.013	1.989	1.00	40.68
ATOM	185	CG2		28	-10.540	63.639	1.672		40.13
ATOM	186		VAL A	28	-12.684	62.844	0.709	1.00	40.08
ATOM		C	VAL A	28	-10.868	61.798		1.00	39.09.
ATOM	187	0	VAL A	28	-9.706	61.381	3.922	1.00	41.23
	188	N	ALA A	29	-11.510		3.963	1.00	41.90
ATOM	189	CA	ALA A	29	-10.854	62.271	4.981	1.00	40.14
ATOM	190	CB	ALA A	29	-11.873	62.492	6.255	1.00	39.42
ATOM	191	C	ALA A			62.936	7.274	1.00	
ATOM	192	0	ALA A		-10.131	61.242	6.731	1.00	40.42
MOTA	193	N		29	-8.963	61.307	7.119		41.63
ATOM	194		GLN A		-10.803	60.099	6.666	1.00	42.66
ATOM	195	CA	GLN A	30	-10.201	58.848	7.106	1.00	44.91
ATOM		CB	GLN A	30	-11.203	57.702	7.106	1.00	48.27
ATOM	196	CG	GLN A	30	-12.400	57.837	6.971	1.00	54.77
	197	CD	GLN A	30	-13.579		7.901	1.00	67.39
ATOM	198	OE1	GLN A		-13.471	56.964	7.495	1.00	75.12
ATOM	199	NE2	GLN A			56.115	6.605	1.00	
ATOM	200		GLN A		-14.724	57.189	8.136	1.00	77.42
ATOM	201			30	-8.930	58.544	6.328		79.26
ATOM	202		GLN A	30	-7.933	58.099	6.898	1.00	47.85
ATOM	203		GLN A	31	-8.972	58.807	5.025	1.00	49.06
ATOM				31	-7.820	58.573		1.00	45.74
ATOM	204	CB	GLN A	31	-8.188	58.781	4.164	1.00	42.76
	205	CG	GLN A	31	-9.129		2.701	1.00	40.15
ATOM	206			31	-9.468	57.723	2.175	1.00	43.01
ATOM	207			31		57.922	0.715	1.00	48.15
ATOM	208				-8.717	57.518	-0.166	1.00	
ATOM	209				-10.609	58.541	0.449	1.00	52.25
ATOM	210			31	-6.675	59.494	4.568		55.93
ATOM	211	-		31	-5.547	59.042	4.765	1.00	41.22
ATOM		_		32	-6.977	60.778	4 732	1.00	43.52
ATOM	212		LE A	32	-5.972	61.746	4.732	1.00	37.48
	213		LE A	32	-6.581	63.140	5.138	1.00	31.13
ATOM	214				-5.615	64.065	5.280	1.00	26.04
ATOM	215					64.067	5.954		22.19
		•		_	-6.987	63.663	3.904		
									25.80

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ATO		216	CD1	ILE A	3.0					
ATO		217	C	ILE A	32	-7.608		39 7 6		
ATO	-1	218	o	ILE A	32	-5.343	61 30			1.00 27.42
ATOM	1	219		ILE A	32	-4.123	61.34	_	58	1.00 34.56
ATOM	1	220	N	ASP A	33	-6.169	60.83		06	9
ATOM			CA	ASP A	33	-5.684				
ATOM		221	CB	ASP A	33	-6.850	60.37	⁵ 8.6		-0.27
ATOM		222		ASP A		-6.380	59.92	9.5		
		223	OD1	ASP A			59.32	8 10 9	-	00 44.05
ATOM		224		ASP A		-5.824	60.066	11.7	77	00 47.52
ATOM		225		ASP A		-6.583	58.111	11.14	-	.00 44.85
ATOM		226	_ •		33 -	4.695	59.233			.00 46.89
ATOM		227		ASP A		3.654	59.209	0.52		.00 36.71
ATOM		228	-	LA A	34 -	5.012	58.285	2.10		.00 39.40
ATOM		229	• • •	LA A		4.129			8 1	22.40
ATOM			CB A	LA A		4.808	57.148	, , 17	5 1	23.00
ATOM		230	C A	LA A		2.783	56.126	6.57		
ATOM		231	O A:	LA A		1.728	57.560	6.84	,	
ATOM		232	N A	LA A			57.088	7.28	`	20.07
	2	233		A A		2.817	58.454	5.851		00 42.04
ATOM	2	234		AA	_	L.596	58.933	5.197		
ATOM	2	235		AA		.941	59.864			00 34.56
ATOM	2	36			35 -0	.697	59.648	4.054		00 31.14
ATOM		37		AA	35 0	.485	59.347	6.189	1.0	33.05
ATOM		38		RΛ	36 -1	.276	60.589	6.295	1.0	36.62
ATOM		39		R A	36 -0	.556	61.369	6.923	1.0	
ATOM				R A		. 503	61.369	7.919	1.0	
ATOM			OG SE				62.396	8.544	1.0	
ATOM			C SEI			.181	63.133	7.539		30.17
	24	12	O SER			054	60.506	9.021	1.0	
ATOM	24	13 j	N ARC			950	60.955	9.750	1.0	
ATOM	24	4 (CA ARG			456	59.288		1.0	0 41.57
ATOM	24	_		_		053	58.394	9.172	1.00	38.47
ATOM	24	_ `			7 -1.	095	57.702	10.191	1.00	38.11
ATOM	24	_ `	G ARG		7 -1.		58.642	10.908	1.00	40.18
ATOM		_	D ARG		7 -3.		50.642	11.805	1.00	10.10
ATOM	24		E ARG		7 -2.9		58.021	12.262	1.00	* 7 . 0 - 2
ATOM	249	_	Z ARG	А 3			56.776	12.976		22.00
	25(H1 ARG		٠. د	359	55.865	13.219	1.00	94.51
ATOM	251	L N	H2 ARG				56.056	12.805	1.00	72.83
ATOM	252		ARG	_			54.753	13.872	1.00	73.10
ATOM	253				0	35	57.393		1.00	79.16
ATOM	254	-	ARG		1.6	77	56.672	9.627	1.00	38.74
ATOM	255		ASP		1.1	51	57.349	10.380	1.00	40.61
ATOM	256						57.349	8.305	1.00	
ATOM				A 38	1.4		56.440	7.658	1.00	40.43
ATOM	257	CG	ASP A	A 38	2.19		55.783	6.437	1.00	41.47
ATOM	258	QD	1 ASP	A 38	2 05		4.556	5.951		49.45
	259	OD	2 ASP		2.82		3.855	6.784	1.00	58.59
ATOM	260	C	ASP A		2.16	2 5	4.281	4.732	1.00	62.36
ATOM	261	0	ASP A		3.35	1 5	7.218	7.262	1.00	62.50
ATOM	262	N			4.21	3 5	7.461		1.00	40.48
ATOM	263		THR A		3.44		7.618	8.105	1.00	36.69
ATOM	264	CA	THR A		4.59		8.376	5.991	1.00	41.01
ATOM	265	CB	THR A	39	4.67	_	0.376	5.480	1.00	
ATOM		0G1		39	3.36		8.298	3.948	1.00	39.22
ATOM	266	CG2	THR A	39	5.223		3.473	3.393	1.00	39.18
ATOM	267	C	THR A	39			.968	3.519		44.29
	268	0	THR A	39	4.497		.847	5.850	1.00	43.28
ATOM	269	N	GLY A		5.505		.538	5.973	1.00	37.79
ATOM	270	CA	GLY A	40	3.268		.323	5.993	1.00	41.79
ATOM	271	С		40	3.038	61	.711	5.333	1.00	35.69
ATOM	272	ō	GLY A	40	2.842	62	.524	6.336	1.00	34.49
ATOM	273		GLY A	40	2.649	63	.735	5.078	1.00	32.99
ATOM	274	N	PHE A	41	2.867	61	. 735	5.153	1.00	35.66
ATOM		CA	PHE A	41	2.713	61	.842	3.932	1.00	
ATOM	275	CB	PHE A	41	3.986	62	.465	2.617	1.00	32.44
ATOM	276	CG	PHE A	41	5.000	62.	260	1.780		30.35
	277	CD1	PHE A	41	5.094	63.	225	2.094	1.00	23.42
ATOM	278	CD2	PHE A		6.079	62.	899	3.013	1.00	19.36
ATOM	279	CE1	PHE A	41	5.161	64.	455	1.454	1.00	19.44
ATOM	280	CE2		41	7.120	63.	790		1.00	20.61
ATOM	281		PHE A	41	6.192	65.	350	3.292	1.00	21.76
ATOM	282	CZ	PHE A	41	7.173	65.	010	1.723	1.00	19.48
ATOM		C	PHE A	41	1.558	O 3 .	0.10	2.642	1.00	
ATOM	283	0	PHE A	41	1.269	61.		1.840	1.00	20.92
ATOM	284	N	PHE A	42	0.900	60.	71	1.988	1.00	30.54
	285	CA	PHE A		0.300	62.6	62	1.016		33.65
ATOM	286	CB	PHE A	42 -	0.179	62.1	.72	0.171	1.00	29.43
ATOM	287	CG .	PHE A	42 -	1.473	61.8	72	0.953	1.00	28.45
ATOM	288	CD1			2.292	63.0		1 222	1.00	28.60
			PHE A	42 -	3.186	63.6	F F	1.332	1.00	26.83
						0		0.431	1.00	26.89

WO 98/16648											
					- 4	6 -				28.60	
					2.218	63.6		.613	1.00	22.24	
* mo:1	289	CD2	PHE A	42 -	3.998	64.7	34	. 803	1.00	28.04	
MOTA MOTA	290	CE1	PHE A		3.030	64.6		2.993	1.00	22.14	
ATOM	291	CE2	PHE A PHE A		-3.919	65.2	• -	2.081 0.979	1.00	30.7	
ATOM	292	CZ	PHE A		-0.416	63.1	2-	0.908	1.00	32.6	
MOTA	293	C	PHE A		-0.046	64.2		2.084	1.00	31.3	
ATOM	294	0	TYR A	43	-0.911	62.5		3.257	1.00	27.2	
MOTA	295	N CA	TYR A	43	-1.200	63.3 62.6	,,,,	4.556	1.00	25.5	
ATOM	296	CB	TYR A	43	-0.851	62.	74.5	5.054	1.00	21.5 19.0	
MOTA	297	CG	TYR A	43	0.573	61.	841	4.942	1.00	17.9	
MOTA	298 299	CD1	TYR A	43	1.524	62.	034	-5.386	1.00	23.5	
MOTA	300	CEl	TYR A	43	2.835 0.966	64.	047	-5.628	1.00 1.00	15.9	91
ATOM	301	CD2	TYR A	43	2.272		246	-6.068	1.00	16.	
ATOM ATOM	302	CE2	TYR A	43	3.198	63.	241	-5.946	1.00	15.	37
ATOM	303	CZ	TYR A	43 43	4.498	63.	456	-6.375	1.00	29.	51
ATOM	304	OH	TYR A	43	-2.673	63	.735	-3.249 -3.163	1.00	26.	3 9
ATOM	305	С	TYR A TYR A	43	-3.528	62	.861	-3.252	1.00	32.	
ATOM	306	0	ALA A	44	-2.96) 65	.026	-3.290	1.00	32.	
ATOM	307	N	ALA A	44	-4.32		.497	-2.586	1.00	31	
MOTA	308	CA CB	ALA A	44	-4.44		.834	-4.769	1.00		.97
MOTA	309	С	ALA A	44	-4.58	٠	.658	-5.414	1.00		. 03
ATOM	310	0	ALA A	44	-3.96		.506 .790	-5.317	1.00		.76 .03
MOTA	311	N	VAL A	45	-5.41		.824	-6.729	1.00		.59
MOTA	312 313	CA	VAL A	45	-5.74	· -	3.440	-7.353	1.00		. 19
MOTA	313	СВ	VAL A		-5.54		2.454	-6.770	1.00		.08
MOTA	315	CG:	1 VAL A		-6.54 -5.6		3.525	-8.861	1.00		5.63
ATOM	316	CG					5.291	-6.866	1.00 1.00		2.25
ATOM	317	C	VAL A		_ ^	•	5.177	-5.917	1.00	3 (5.71
MOTA MOTA	318	0	VAL A			38 6	5.823	-8.034	1.00	3	5.51
ATOM	319	N	ASN A	•		.83 6	6.349	-8.294	1.00		2.00
ATOM	320	CP	- 637			156 6	5.320	-7.942 -9.144	1.00	5	1.81
ATOM	321			•		36	4.547	-9.671	1.00		8.83
MOTA	322					113	64.813	-9.588	1.00		4.06
ATOM	323			••	6 -9.	641	63.582	-7.494	1.00		2.25
ATOM	324			• •	6 -9.		67.618	-6.996	1.00		35.38
MOTA	325	_	* 617	A 4	6 -10.		67.848 68.452	-7.409	1.00		34.05 34.39
MOTA	326	·		A 4		093	69.718	-6.659	1.00		29.40
MOTA	32° 32	´ -	A HIS	A 4		106	70.088	-6.306	1.00	•	26.18
MOTA	32	٠.	B HIS	A 4	•	674	69.842	-7.425	1.00	•	27.13
MOTA	33	· .	CG HIS			.716 .906	68.789	-7.686	1.00	,	29.56
MOTA	33		CD2 HIS		-	. 573	70.709	-8.486	1.0		29.92
ATOM	33		ND1 HIS			.717	70.199	-9.355	1.0		29.91
ATOM ATOM	3 3	13	CE1 HIS			.299	69.034	-8.894	1.0		35.30
MOTA	3.3	3 4	NE2 HIS			.740	70.890	-7.397 -6.825	1.0		36.82
ATOM	3	3 5		A a		.889	71.972	-8.700	1.0		36.56
ATOM	3	36		ΥA		.955	70.710	-9.528	1.0	00	37.05
MOTA		37	**	Y A		9.578	71.732	-9.879	1.		40.00
ATOM		38		A Y		3.759	72.959 74.004	-10.196	1.		46.68
MOTA		39	-	A Y		9.321	72.819	-9.913	1.		37.89 36.05
MOTA		40		EΑ		7.440	73.948	-10.220	1.		31.81
MOTA		341 342		EΑ		6.568	74.191	-9.082		00	28.58
MOTA		343		LE A		5.546	75.255	-9.488	_	00	29.79
MOTA		344	CG2 I	LE A		4.522	74.596	-7.807		.00	32.52
MOTA		345		LE A		-5.425	74.629	-6.574	•	.00	38.13
ATOM		346	C= -	LE A		-5.815	73.686	-11.514	•	.00	38.18
MOTA MOTA		347		LE A		-5.297	72.581	-11.70		.00	38.60
MOTA		348		LE A		-5.749	74.701	-12.38	•	.00	38.30
ATOM		349		SN A		-5.050	74.603		5	.00	42.37
ATOM		350	· · · ·	ASN A ASN A	50	-5.453	75.726	2 (03	,	. 00	46.03
ATOM		351			50	-4.920	75.502	1 (21	-	L.00	46.67
ATON		352		ASN A ASN A	50	-4.258	74.496	10 00	22	1.00	49.68
ATO		353	-	ASN A	50	-5.195	76.445	4	39	1.00	38.19
OTA		354	ND2 C	ASN A	50	-3.544	74.614		81	1.00	36.43
ATO	М	355	0	ASN A	50	-2.853	75.633 73.430	-13.0	86	1.00	39.42
ATO		356	N	VAL A	51	-3.064	73.43	5 -12.7	86	1.00	38.94 36.89
OTA		357	CA	VAL A	51	-1.676	-4 77	4 -12.1	82	1.00	39.25
ATO		358 359	CB	VAL A	51	-1.582		-13.0	40	1.00	37.13
ATC		360	CG1	VAL A		-0.757 -1.103	22 70		156	1.00	• = -
)TA		361	CG2	VAL A	. 51	-1.103					
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NTOM	362	С	VAL A	51	-0.804	73.346	-14.025	1.00	40.42
ATOM ATOM	363	0	VAL A	51	0.370	73.688	-13.923	1.00	40.47
ATOM	364	N	GLN A	52	-1.404	73.193	-15.198	1.00	43.48
ATOM	365	CA	GLN A	52	-0.658	73.335	-16.439	1.00	46.46
MOTA	366	CB	GLN A	52	-1.461	72.753	-17.607	1.00	54.80
MOTA	367	CG	GLN A	52	-1.828	71.265	-17.427	1.00	64.12
ATOM	368	CD	GLN A	52	-0.603	70.340	-17.338	1.00	70.98
ATOM	369	OE1	GLN A	52	0.494	70.696	-17.774 -16.788	1.00 1.00	73.27 71.68
MOTA	370	NE2 C	GLN A GLN A	52 52	-0.799 -0.250	69.140 74.787	-16.783	1.00	42.90
MOTA MOTA	371 372	0	GLN A	52	0.932	75.081	-16.876	1.00	42.08
ATOM	373	N	ARG A	53	-1.212	75.704	-16.649	1.00	40.10
ATOM	374	CA	ARG A	53	-0.902	77.119	-16.860	1.00	40.21
MOTA	375	CB	ARG A	53	-2.161	77.981	-16.766	1.00	39.62
ATOM	376	CG	ARG A	53	-1.896	79.468	-16.979	1.00	46.56
MOTA	377	CD	ARG A	53	-3.084	80.302	-16.558	1.00	55.52
ATOM	378	NE	ARG A	53	-3.456	80.002	-15.180	1.00	69.72
ATOM	379	CZ	ARG A	53	-4.707	79.854 79.988	-14.750 -15.589	1.00	75.43 79.20
ATOM	380	NH1 NH2	ARG A ARG A	53 53	-5. 72 8 -4.936	79.529	-13.485	1.00	80.30
MOTA MOTA	381 382	C	ARG A	53	0.112	77.592	-15.818	1.00	40.89
ATOM	383	0	ARG A	53	0.967	78.436	-16.103	1.00	42.68
ATOM	384	N	LEU A	54	0.015	77.025	-14.617	1.00	40.83
ATOM	385	CA	LEU A	54	0.906	77.354	-13.513	1.00	36.14
ATOM	386	CB	LEU A	54	0.481	76.583	-12.263	1.00	36.52
ATOM	387	CG	LEU A	54	1.431	76.620	-11.068	1.00	35.31
MOTA	388	CD1	LEU A	54	1.581	78.057	-10.586	1.00	33.45
ATOM	389	CD2	LEU A	54	0.904	75. 71 0 77.073	-9.969 -13.829	1.00	36.19 36.31
ATOM	390	C	LEU A LEU A	54 54	2.380 3.231	77.935	-13.618	1.00	37.16
ATOM ATOM	391 392	O N	SER A	55	2.695	75.883	-14.335	1.00	34.98
ATOM	393	CA	SER A	55	4.090	75.558	-14.645	1.00	36.10
ATOM	394	CB	SER A	55	4.261	74.066	-14.929	1.00	32.09
ATOM	395	og	SER A	55	3.071	73.521	-15.455	1.00	41.05
ATOM	396	С	SER A	55	4.618	76.377	-15.804	1.00	37.67
ATOM	397	0	SER A	55	5. 78 9	76.752	-15.825	1.00	41.07
ATOM	398	N	GLN A	56	3.740	76.688	-16.744	1.00 1.00	37.35 38.51
ATOM	399	CA	GLN A GLN A	56 56	4.105 2.940	77.460 77.439	-17.9 1 9 -18.902	1.00	46.09
ATOM	400 401	CB CG	GLN A	56	3.138	78.188	-20.191	1.00	58.62
ATOM ATOM	402	CD	GLN A	56	1.811	78.422	-20.902	1.00	71.60
ATOM	403	OE1	GLN A	56	1.007	77.494	-21.071	1.00	75.28
ATOM	404	NE2	GLN A	56	1.560	79.672	-21.296	1.00	74.89
ATOM	405	С	GLN A	56	4.496	78.893	-17.560	1.00	36.41
MOTA	406	0	GLN A	56	5.611	79.312	-17.848	1.00	35.97
MOTA	407	N	LYS A	57	3.599	79.629	-16.905	1.00	35.19 34.22
ATOM	408	CA	LYS A LYS A	57 57	3.869 2. 710	81.015 81.567	-16.514 -15.693	1.00 1.00	35.10
ATOM	409 410	CB CG	LYS A	57	1.443	81.768	-16.469	1.00	41.47
ATOM ATOM	411	CD	LYS A	57	1.644	82.849	-17.492	1.00	49.86
ATOM	412	CE	LYS A	57	0.507	82.868	-18.477	1.00	58.96
ATOM	413	NZ	LYS A	57	0.740	83.914	-19.507	1.00	67.82
ATOM	414	С	LYS A	5 7	5.147	81.106	-15.691	1.00	36.94
ATOM	415	0	LYS A	57	5.963	82.014	-15.875	1.00	38.60
ATOM	416	N	THR A	58	5.277	80.172	-14.753	1.00	37.65
ATOM	417	CA	THR A	58	6.426	80.066	-13.865	1.00	35.48 36.09
ATOM	418	CB	THR A	58	6.215 5.257	78.911 79.317	-12.846 -11.862	1.00	30.91
MOTA	419	OG1 CG2	THR A THR A	58 58	7.503	78.549	-12.142	1.00	43.44
ATOM ATOM	420 421	C	THR A	58	7.696	79.833	-14.665	1.00	35.79
MOTA	422	0	THR A	58	8.686	80.531	-14.463	1.00	37.07
ATOM	423	N	LYS A	59	7.667	78.865	-15.577	1.00	38.20
ATOM	424	CA	LYS A	59	8.832	78.573	-16.397	1.00	40.23
ATOM	425	CB	LYS A	59	8.540	77.444	-17.391	1.00	46.70
ATOM	426	CG	LYS A	59	9.744	77.071	-18.254	1.00	58.45
ATOM	427	CD	LYS A	59	9.534	75.783	-19.053	1.00	69.21
ATOM	428	CE	LYS A	59	10.831	75.350	-19.769 -20.510	1.00	76.48 75.66
ATOM	429	NZ	LYS A	59 59	10. 728 9. 19 9	74.041 79.846	-17.134	1.00	40.20
ATOM	430	C 0	LYS A LYS A	59 59	10.364	80.239	-17.167	1.00	41.89
ATOM ATOM	431 432	N	GLU A	60	8.186	80.531	-17.653	1.00	41.30
MOTA	432	CA	GLU A	60	8.395	81.777	-18.379	1.00	42.90
ATOM	434	CB	GLU A	60	7.059	82.362	-18.851	1.00	50.15

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ATOM	435	CG	GLU A	60	6.405	81.626	-20.026	1.00	57.31
ATOM	436	CD	GLU A	60	5.215	82.383	-20.605	1.00	63.82
ATOM	437	OE1	GLU A	60	4.233	81.733	-21.027	1.00	68.21
ATOM	438	OE2	GLU A	60	5.259	83.633	-20.644	1.00	67.21
ATOM	439	C	GLU A	60	9.115	82.773	-17.484	1.00	39.96
MOTA	440	0	GLU A	60	10.147	83.324	-17.859	1.00	42.99
ATOM	441	N	PHE A	61	8.604	82.949	-16.274	1.00	35.82
ATOM ATOM	442 443	CA CB	PHE A PHE A	61	9.208	83.874	-15.325	1.00	34.12
ATOM	444	CG	PHE A	61 61	8.466 9.039	83.810 84.718	-13.978 -12.918	1.00	30.54
ATOM	445	CD1	PHE A	61	8.905	86.093	-13.013	1.00	25.45 20.40
ATOM	446	CD2	PHE A	61	9.730	84.193	-11.835	1.00	23.25
MOTA	447	CE1	PHE A	61	9.449	86.928	-12.053	1.00	19.57
ATOM	448	CE2	PHE A	61	10.277	85.026	-10.875	1.00	22.69
ATOM	449	CZ	PHE A	61	10.133	86.399	-10.989	1.00	17.25
ATOM	450	С	PHE A	61	10.710	83.620	-15.115	1.00	32.38
ATOM	451	0	PHE A	61	11.536	84.499	-15.353	1.00	30.20
ATOM	452	N	HIS A	62	11.064	82.407	-14.714	1.00	34.34
ATOM ATOM	453	CA CB	HIS A HIS A	62	12.458	82.076	-14.436	1.00	37.14
ATOM	454 455	CG	HIS A	62 62	12.556 12.181	80.693 80.696	-13.779 -12.331	1.00	32.21
ATOM	456	CD2	HIS A	62	11.234	80.007	-11.652	1.00	31.98 29.94
ATOM	457	ND1	HIS A	62	12.792	81.519	-11.410	1.00	28.87
ATOM	458	CE1	HIS A	62	12.234	81.344	-10.228	1.00	28.92
ATOM	459	NE2	HIS A	62	11.286	80.432	-10.347	1.00	29.72
ATOM	460	C	HIS A	62	13.437	82.193	-15.599	1.00	41.35
MOTA	461	0	HIS A	62	14.604	82.546	-15.405	1.00	40.97
MOTA	462	N	MET A	63	12.968	81.941	-16.809	1.00	43.02
ATOM	463	CA	MET A	63	13.867	82.018	-17.941	1.00	45.13
ATOM	464	CB	MET A	63	13.396	81.102	-19.070	1.00	51.35
ATOM	465	CG	MET A	63	13.180	79.653	-18.631	1.00	63.00
ATOM ATOM	466 467	SD CE	MET A MET A	63	14.560	78.941	-17.665	1.00	73.59
ATOM	463	C	MET A	63 63	15.229 14.052	77.786 83.438	-18.858 -18.445	1.00	73.56
ATOM	469	0	MET A	63	15.126	83.781	-18.927	1.00 1.00	44.26 50.29
ATOM	470	N	SER A	64	13.041	84.283	-18.287	1.00	39.05
ATOM	471	CA	SER A	64	13.133	85.648	-18.782	1.00	36.67
ATOM	472	CB	SER A	64	11.798	86.062	-19.386	1.00	37.55
ATOM	473	OG	SER A	64	10.763	86.008	-18.428	1.00	43.44
MOTA	474	С	SER A	64	13.611	86.739	-17.837	1.00	39.95
ATOM	475	0	SER A	64	14.019	87.806	-18.296	1.00	45.98
ATOM	476	N	ILE A	65	13.486	86.531	-16.530	1.00	41.66
ATOM	477	CA	ILE A	65	13.914	87.547	-15.568	1.00	37.23
ATOM ATOM	478 479	CB	ILE A	65	13.477	87.209	-14.108	1.00	35.14
ATOM	480	CG2 CG1	ILE A ILE A	65 65	14.228 13.725	86.007 88.412	-13.559	1.00	26.54
ATOM	481	CD1	ILE A	65	12.960	88.365	-13.207 -11.914	1.00 1.00	31.65 37.39
ATOM	482	C	ILE A	65	15.420	87.732	-15.672	1.00	38.75
ATOM	483	0	ILE A	65	16.165	86.757	-15.710	1.00	43.09
ATOM	484	N	THR A	66	15.857	88.980	-15.785	1.00	38.80
MOTA	485	CA	THR A	66	17.278	89.281	-15.924	1.00	39.81
ATOM	486	CB	THR A	66	17.486	90.544	-16.776	1.00	40.56
ATOM	487	OG1	THR A	66	16.886	91.663	-16.113	1.00	47.40
MOTA	488	CG2	THR A	66	16.854	90.371	-18.139	1.00	41.17
ATOM	489	C	THR A	66	17.948	89.502	-14.580	1.00	39.84
ATOM	490	0	THR A PRO A	66	17.291	89.829	-13.597	1.00	46.85
ATOM ATOM	491 492	N CD	PRO A	67 67	19.279 20.152	89.365	-14.524	1.00	40.14
ATOM	493	CA	PRO A	67	20.132	88.850 89.557	-15.590 -13.281	1.00 1.00	39.50
ATOM	494	CB	PRO A	67	21.482	89.273	-13.281	1.00	39.40 39.30
ATOM	495	CG	PRO A	67	21.459	89.446	-15.212	1.00	40.61
ATOM	496	С	PRO A	67	19.884	90.924	-12.604	1.00	39.27
ATOM	497	0	PRO A	67	19.934	91.012	-11.378	1.00	42.45
ATOM	498	N	GLU A	68	19.704	91.986	-13.387	1.00	37.98
ATOM	499	CA	GLU A	68	19.528	93.316	-12.811	1.00	36.08
ATOM	500	CB	GLU A	68	19.598	94.425	-13.865	1.00	44.41
ATOM	501	CG	GLU A	68	20.830	94.408	-14.745	1.00	56.01
ATOM	502	CD	GLU A	68	20.701	93.426	-15.897	1.00	62.86
ATOM	503	OE1	GLU A	68	19.776	93.599	-16.727	1.00	65.53
ATOM ATOM	504 505	OE2	GLU A GLU A	68	21.519	92.480	-15.972	1.00	66.08
ATOM	505 506	C .	GLU A	68 68	18.166	93.349	-12.157	1.00	32.92
ATOM	507	N	GLU A	69	17.968 17.217	94.037 92.633	-11.158 -12.747	1.00	37.34
	50.		020 A	9,5	11.211	J2.033	- 12. /7/	1.00	28.56

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			CI II A	69	15.877	92.560	-12.193	1.00	26.48
ATOM	508	CA CB	GLU A GLU A		14.927	91.889	-13.170	1.00	26.48
MOTA	509	CG	GLU A		14.696	92.647	-14.438	1.00	31.14
ATOM	510 511	CD	GLU A		13.480	92.145	-15.147	1.00	36.47
ATOM	512	OE1	GLU A	69	12.386	92.682	-14.875	1.00	41.34
ATOM ATOM	513	OE2	GLU A	69	13.612	91.195	-15.946	1.00	41.53 26.61
ATOM	514	С	GLU A	69	15.925	91.749	-10.900	1.00	33.09
ATOM	515	0	GLU A		15.268	92.086	-9.916	1.00 1.00	23.31
ATOM	516	N	LYS A		16.703	90.672	-10.902	1.00	18.07
ATOM	517	CA	LYS A		16.830	89.844	-9.719 -10.000	1.00	16.10
ATOM	518	CB	LYS A		17.730	88.655 87.693	-10.000	1.00	16.50
MOTA	519	CG	LYS A		17.125	86.602	-11.323	1.00	19.40
ATOM	520	CD	LYS A	70	18.081 17.421	85.611	-12.243	1.00	23.23
MOTA	521	CE	LYS A	70 70	18.372	84.538	-12.604	1.00	28.38
ATOM	522	NZ	LYS A LYS A	70	17.397	90.685	-8.596	1.00	22.66
MOTA	523	С 0	LYS A	70	16.836	90.725	-7.505	1.00	27.15
MOTA	524 525	Ŋ	TRP A	71	18.461	91.424	-8.891	1.00	21.96
ATOM	525	CA	TRP A	71	19.101	92.274	-7.897	1.00	22.52
ATOM	527	CB	TRP A	71	20.321	92.982	-8.494	1.00	19.42
ATOM ATOM	528	CG	TRP A	71	21.037	93.865	-7.506	1.00	20.03 17.51
ATOM	529	CD2	TRP A	71	21.800	93.441	-6.366	1.00	15.91
ATOM	530	CE2	TRP A	71	22.293	94.604	-5.736	1.00	19.70
ATOM	531	CE3	TRP A	71	22.103	92.194	-5.809 -7.524	1.00	18.18
ATOM	532	CD1	TRP A	71	21.104	95.230 95.680	-6.466	1.00	21.55
ATOM	533	NE1	TRP A	71	21.859	94.559	-4.585	1.00	20.06
ATOM	534	CZ2	TRP A	71	23.089 22.897	92.147	-4.662	1.00	20.49
MOTA	535	CZ3	TRP A	71 71	23.373	93.324	-4.061	1.00	20.53
MOTA	536	CH2	TRP A TRP A	71	18.123	93.299	-7.359	1.00	23.60
ATOM	537	C 0	TRP A	71	18.089	93.584	-6.155	1.00	24.12
ATOM	538 539	И	ASP A	72	17.327	93.860	-8.254	1.00	23.56
ATOM	540	CA	ASP A	72	16.358	94.859	7.860	1.00	27.03
ATOM	541	CB	ASP A	72	15.853	95.630	-9.083	1.00	34.54
ATOM ATOM	542	CG	ASP A	72	16.921	96.534	-9.692	1.00	40.55 47.37
ATOM	543	OD1	ASP A	72	18.116	96.375	-9.363	1.00 1.00	50.79
ATOM	544	OD2	ASP A	72	16.563	97.416	-10.502	1.00	26.53
ATOM	545	С	ASP A	72	15.208	94.309	-7.032 -6.384	1.00	33.99
ATOM	546	0	ASP A	72	14.506	95.082	-6.999	1.00	23.44
ATOM	547	N	LEU A	73	15.055	92.989 92.353	-6.224	1.00	19.61
ATOM	548	CA	LEU A	73	13.998 13.219	91.372	-7.091	1.00	20.50
ATOM	549	CB	LEU A	73 73	12.333	91.920	-8.201	1.00	20.73
MOTA	550	CG	LEU A LEU A	73	11.692	90.760	-8.945	1.00	10.89
MOTA	551	CD1 CD2	LEU A	73	11.280	92.830	-7.601	1.00	14.36
ATOM	552 553	C	LEU A	73	14.558	91.581	-5.049	1.00	19.51
ATOM	554	o	LEU A	73	13.811	91.098	-4.212	1.00	22.35
ATOM	555	N	ALA A	74	15.871	91.415	-5.019	1.00	20.26
ATOM ATOM	556	CA	ALA A	74	16.535	90.656	-3.965	1.00	18.26 17.07
ATOM	557	СВ	ALA A	74	18.046	90.726	-4.146	1.00 1.00	19.57
ATOM	558	С	ALA A	74	16.163	91.106	-2.569 -2.344	1.00	17.06
MOTA	559	0	ALA A	74	15.917	92.285 90.157	-1.637	1.00	21.97
MOTA	560	N	ILE A	75	16.115	90.157	-0.239	1.00	18.37
MOTA	561	CA	ILE A	75	15.811 15.337	89.202	0.514	1.00	15.88
MOTA	562	CB	ILE A	75 75	14.056	88.700	-0.073	1.00	15.90
MOTA	563	CG2		75 75	16.380	88.096	0.422	1.00	17.42
ATOM	564	CG1 CD1		75	16.178	86.992	1.424	1.00	20.14
ATOM	565 566	C	ILE A	75	17.051	91.063	0.453	1.00	22.26
ATOM	566 567	0	ILE A	75		91.028	-0.093	1.00	24.15
MOTA	568	N	ARG A	76		91.598	1.656	1.00	23.62
ATOM ATOM	569	CA	ARG A	76	17.934	92.244	2.423	1.00	22.51
ATOM	570	СВ	ARG A	76	17.382	-92.683	3.776	1.00	25.41 30.98
ATOM	571	CG	ARG A	76		93.622	4.540	1.00	39.61
ATOM	572	CD	ARG A				5.878	1.00 1.00	43.97
MOTA	573	NE	ARG A				6.731 7.719	1.00	46.12
MOTA	574	CZ					7.719	1.00	44.59
ATOM	575	NH					8.417	1.00	44.99
ATOM	576	NH					2.622	1.00	20.90
ATOM	577	C	ARG A				2.667	1.00	21.19
ATOM	578	0	ARG A				2.773	1.00	22.00
MOTA	579	N CA	ALA A ALA A				2.962	1.00	20.40
MOTA	580	CA		•					

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ATOM	581	СВ	ALA A	. 77	19.706	87.798	3.239	1 00	
ATOM	582	C	ALA A			89.245	1.770	1.00 1.00	16.39
ATOM ATOM	583	0	ALA A		22.275	88.824	1.889	1.00	24.32 29.02
ATOM	584	N	TYR A			89.704	0.618	1.00	25.02
ATOM	585 586	CA CB	TYR A			89.795	-0.587	1.00	19.05
ATOM	587	CB	TYR A	78		89.103	-1.764	1.00	16.11
ATOM	588	CD1	TYR A TYR A	78 78		87.618	-1.613	1.00	16.70
ATOM	589	CE1		78	19.611 19.542	87.000	-1.114	1.00	15.71
ATOM	590	CD2		78	21.821	85.626 86.823	-1.006	1.00	14.79
MOTA	591	CE2		78	21.762	85.458	-1.987 -1.886	1.00	17.98
ATOM	592	CZ	TYR A	78	20.624	84.864	-1.394	1.00	15.81
ATOM	593	OH	TYR A	78	20.563	83.495	-1.336	1.00	19.26
ATOM ATOM	594	C	TYR A	78	21.735	91.233	-0.952	1.00	27.92 18.90
ATOM	595 596	0	TYR A	78	22.874	91.609	-1.178	1.00	24.83
ATOM	597	N CA	ASN A	79	20.672	92.025	-1.046	1.00	20.12
ATOM	598	CB	ASN A ASN A	79	20.778	93.442	-1.396	1.00	23.74
ATOM	599	CG	ASN A	79 79	19.767 19.985	93.794	-2.491	1.00	21.09
ATOM	600	OD1	ASN A	79	20.558	95.173 96.049	-3.071	1.00	20.38
ATOM	601	ND2	ASN A	79	19.511	95.378	-2.437	1.00	24.59
ATOM	602	С	ASN A	79	20.563	94.310	-4.283 -0.161	1.00	17.81
ATOM	603	0	ASN A	79	19.442	94.645	0.206	1.00	26.18
ATOM	604	N	LYS A	80	21.668	94.695	0.452	1.00	28.37
ATOM ATOM	605	CA	LYS A	80	21.693	95.496	1.663	1.00	28.39 28.15
ATOM	606 607	CB	LYS A	80	23.145	95.869	1.926	1.00	30.31
ATOM	608	CG CD	LYS A LYS A	80	23.434	96.446	3.270	1.00	41.68
ATOM	609	CE	LYS A	80 80	24.934	96.530	3.472	1.00	49.85
ATOM	610	NZ	LYS A	80	25.290 26.764	97.287	4.739	1.00	56.09
ATOM	611	С	LYS A	80	20.805	97.261 96.741	4.971	1.00	59.86
ATOM	612	0	LYS A	80	20.388	97.234	1.640	1.00	28.30
ATOM	613	N	GLU A	81	20.444	97.183	2.679 0.448	1.00	31.85
ATOM	614	CA	GLU A	81	19.631	98.377	0.245	1.00	27.68
ATOM	615	CB	GLU A	81	19.700	98.738	-1.245	1.00	27.82 26.85
ATOM ATOM	616	CG	GLU A	81	18.936	99.974	-1.667	1.00	25.54
ATOM	617 618	CD	GLU A	81	18.843	100.115	-3.173	1.00	27.23
ATOM	619	OE1 OE2	GLU A GLU A	81	18.424	101.187	-3.645	1.00	30.11
ATOM	620	C	GLU A	81	19.177	99.153	-3.892	1.00	35.72
ATOM	621	ō	GLU A	81 81	18.163 17.592	98.261	0.685	1.00	28.54
ATOM	622	N	HIS A	82	17.544	99.190 97.125	1.260	1.00	32.85
ATOM	623	CA	HIS A	82	16.145	96.919	0.400 0.736	1.00	28.51
ATOM	624	CB	HIS A	82	15.547	95.839	-0.148	1.00	26.34
ATOM	625	CG	HIS A	82	15.992	95.898	-1.569	1.00	23.16 20.08
ATOM ATOM	626	CD2	HIS A	82	16.006	96.906	-2.467	1.00	14.88
ATOM	627 628	ND1	HIS A	82	16.428	94.781	-2.241	1.00	21.04
ATOM	629	CE1 NE2	HIS A	82	16.684	95.094	-3.493	1.00	20.58
ATOM	630	C	HIS A HIS A	82	16.433	96.382	-3.661	1.00	16.40
ATOM	631	0	HIS A	82 82	15.992	96.461	2.168	1.00	29.32
ATOM	632	N	GLN A	83	15.653 16.193	95.302 97.366	2.415	1.00	29.56
MOTA	633	CA	GLN A	83	16.084	97.006	3.113 4.517	1.00	32.90
ATOM	634	CB	GLN A	83	16.438	98.194	5.406	1.00	36.06
ATOM	635	CG	GLN A	83	17.942	98.406	5.566	1.00	42.46
ATOM	636	CD	GLN A	83	18.637	97.224	6.227	1.00	54.39 60.00
ATOM ATOM	637	OE1	GLN A	83	18.366	96.899	7.386	1.00	66.86
ATOM	638 639	NE2	GLN A	83	19.534	96.572	5.492	1.00	60.20
ATOM	640	C 0	GLN A	83	14.746	96.418	4.932	1.00	34.12
ATOM	641	N	GLN A ASP A	83 84	14.689	95.623	5.856	1.00	36.75
ATOM	642	CA	ASP A		13.684 12.353	96.755	4.215	1.00	35.26
MOTA	643	СВ	ASP A		11.293	96.260	4.546	1.00	35.02
ATOM	644	CG	ASP A		11.437	97.298 98.611	4.158	1.00	47.91
ATOM	645	OD1	ASP A		11.115	99.673	4.925 4.344	1.00	61.72
ATOM	646	OD2	ASP A		11.863	98.587	6.104	1.00	68.07
ATOM	647	С	ASP A		11.987	94.912	3.931	1.00	69.22
ATOM	648	0	ASP A	84	10.890	94.402	4.158	1.00	30.42 31.96
MOTA MOTA	649 650	N	GLN A		12.881	94.331	3.146	1.00	23.30
ATOM	650 651	CA	GLN A		12.571	93.058	2.537	1.00	20.72
ATOM	652	CB CG	GLN A GLN A		12.946	93.059	1.068	1.00	20.88
ATOM	653	CD	GLN A		12.181	94.019	0.236	1.00	23.30
			· A	J	12.434	93.811	-1.235	1.00	32.07

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						2. 7.52	-1.982	1.00	41.87
MOTA	654	QE1 G			12.670	94.762	-1.666	1.00	31.81
ATOM	655	NE2 G			12.378	92.565	3.242	1.00	22.01
	656	C G	LN A		13.286	91.930	3.061	1.00	25.61
ATOM	657		LN A		14.485	91.736	4.038	1.00	21.04
ATOM	658		AL A		12.551	91.171	4.758	1.00	20.72
ATOM	659		/AL A	86	13.151	90.063		1.00	23.91
MOTA	660		/AL A	86	12.835	90.127	6.271 6.993	1.00	24.41
ATOM	661		/AL A		13.522	88.996		1.00	24.17
MOTA	662		JAL A	86	13.272	91.445	6.856	1.00	20.58
ATOM			VAL A	86	12.717	88.713	4.204	1.00	29.31
MOTA	663	-	VAL A	86	13.554	87.851	3.990	1.00	18.86
ATOM	664	-	ARG A	87	11.417	88.530	3.990		18.95
MOTA	665		ARG A		10.875	87.270	3.467	1.00	21.46
MOTA	666		ARG A	87	9.560	86.885	4.153	1.00	24.00
MOTA	667		ARG A	87	9.591	86.566	5.630	1.00	
ATOM	668		ARG A	87	8.153	86.365	6.142	1.00	23.85
ATOM	669			87	7.549	85.127	5.647	1.00	26.86
MOTA	670	•	ARG A	87	6.252	84.833	5.742	1.00	24.59
ATOM	671		ARG A	87	5.412	85.691	6.300	1.00	22.47
MOTA	672	NH1	ARG A	87	5.803	83.654	5.333	1.00	22.94
ATOM	673	NH2	ARG A		10.548	87.409	1.989	1.00	17.44
ATOM	674	C	ARG A	87		86.591	1.181	1.00	20.34
ATOM	675	0	ARG A	87	10.947	88.456	1.657	1.00	14.27
MOTA	676	И	ALA A	88	9.803	88.708	0.296	1.00	15.50
MOTA	677	CA	ALA A	88	9.353	89.637	0.307	1.00	11.55
ATOM	678	CB	ALA A	88	8.154		-0.630	1.00	18.22
ATOM	679	С	ALA A	88	10.413	89.247 90.190	-0.284	1.00	24.16
ATOM	680	0	ALA A	88	11.122		-1.837	1.00	18.31
ATOM	681	N	GLY A	89	10.461	88.688	-2.825	1.00	18.37
	682	CA	GLY A	89	11.437	89.103	-3.422	1.00	21.93
MOTA	683	С	GLY A	89	12.221	87.946	-3.422	1.00	23.18
ATOM	684	0	GLY A	89	11.853	86.773		1.00	21.46
MOTA	685	N	TYR A	90	13.315	88.286	-4.103	1.00	17.61
MOTA	686	CA	TYR A	90	14.178	87.314	-4.767	1.00	14.11
ATOM		CB	TYR A	90	14.701	87.909	-6.098	1.00	15.32
ATOM	687	CG	TYR A	90	14.847	86.895	-7.215	1.00	15.35
ATOM	688	CD1	TYR A	90	13.827	86.705	-8.142		17.27
ATOM	689		TYR A	90	13.900	85.686	-9.100	1.00	17.90
MOTA	690	CE1	TYR A	90	15.963	86.050	-7.283	1.00	18.10
ATOM	691	CD2	TYR A	90	16.047	85.031	-8.236	1.00	
MOTA '	692	CE2	TYR A	90	15.010	84.855	-9.136	1.00	18.33
MOTA	693	CZ		90	15.056	83.829	-10.056	1.00	29.46
ATOM	694	OH	TYR A	90	15.344	86.861	-3.881	1.00	18.14
MOTA	695	С	TYR A		15.877	87.636	-3.089	1.00	19.67
MOTA	696	0	TYR A	90	15.713	85.592	-4.013	1.00	20.08
MOTA	697	N	TYR A	91	16.819	84.976	-3.277	1.00	20.39
ATOM	698	CA	TYR A	91		83.713	-2.542	1.00	20.44
ATOM	699	CB	TYR A	91	16.354	83.965	-1.432	1.00	20.34
MOTA	700	CG	TYR A	91		84.566	-1.693	1.00	21.65
MOTA	701	CD1	TYR A	91			-0.677	1.00	16.23
ATOM	702	CEl	TYR A	91		84.819	-0.120	1.00	18.42
ATOM	703	CD2	TYR A	91		83.622	0.898	1.00	20.40
ATOM	704	CE2	TYR A	91		83.867	0.615	1.00	22.22
	705	CZ	TYR A	91		84.468	1.639	1.00	21.37
ATOM	706	OH	TYR A	91		84.705		1.00	23.73
MOTA	707	c	TYR A	91	L 17.819	84.603	-4.362	1.00	24.20
MOTA		0	TYR A	9:	17.583	83.687	-5.154	1.00	28.01
MOTA	708	N	LEU A		2 18.894	85.374	-4.451		24.96
ATOM	709		LEU A	_		85.160	-5.476	1.00	24.17
MOTA	710	CA	LEU A				-5.534	1.00	19.59
MOTA	711	CB					-5.635	1.00	
MOTA	712		LEU A	_			-5.696	1.00	23.44
MOTA	713						-6.850	1.00	22.64
MOTA	714	CD2					-5.283	1.00	25.80
ATOM	715	C	LEU A		·		-4.174	1.00	25.07
ATOM	716		LEU P		2 20.879			1.00	26.00
ATOM	717	_	SER A	_	3 21.31			1.00	27.05
ATOM	718		SER A		3 22.21			1.00	24.34
	719		SER I	Α 9	22.21			1.00	26.84
ATOM	720		SER	Α. 9	22.43			1.00	27.46
MOTA	72	_	SER A		93 23.56			1.00	26.92
ATOM			SER		93 23.77			1.00	29.65
MOTA	723	<u>.</u>	ILE		94 24.48			1.00	31.96
MOTA	72				94 25.79	7 82.716			33.15
MOTA	72	-	·		94 26.10	6 82.624	~	1.00	29.48
ATOM	72				94 27.46		-3.456	1.00	23.40
MOTA	72	۰ د		-					

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ATOM	72	7 CG	1 ILE A	A 94	1 25 025				
ATOM	728						-2.946	1.00	33.35
ATOM	729		ILE A				-1.463	1.00	36.58
ATOM	730	0	ILE A				-6.027	1.00	34.38
ATOM	731	L N	PRO A				-5.717	1.00	36.74
ATOM	732		PRO A				-7.080	1.00	38.50
ATOM	733	CA	PRO A				-7.350	1.00	40.61
ATOM	734		PRO A			81.724	-7.947	1.00	40.90
ATOM	735		PRO A			82.854	-8.745	1.00	45.71
ATOM	736		PRO A	_		84.049	-7.829	1.00	45.59
ATOM	737		PRO A		29.309	80.929	-7.159	1.00	39.51
ATOM	738		GLY A	96	30.004	81.477	-6.310	1.00	42.47
ATOM	739		GLY A	96	29.327	79.625	-7.391	1.00	38.51
ATOM	740	С	GLY A	96	30.259	78.752	-6.713	1.00	35.63
ATOM	741	0	GLY A	96	29.740	78.161	-5.424	1.00	37.97
ATOM	742	N	LYS A	97	30.126	77.062	-5.047	1.00	39.52
ATOM	743	CA	LYS A	97	28.812	78.849	-4.777	1.00	35.33
ATOM	744	СВ	LYS A	97	28.318	78.365	-3.504	1.00	34.40
ATOM	745	CG	LYS A	97	28.555	79.419	-2.435	1.00	42.78
ATOM	746	CD	LYS A	97	29.982	79.900	-2.352	1.00	54.46
ATOM	747	CE	LYS A	97	30.041	81.101	-1.428	1.00	65.72
ATOM	748	NZ	LYS A	97	31.450	81.651	-1.284	1.00	73.04
ATOM	749	C	LYS A	97	31.498	82.894	-0.447	1.00	78.91
ATOM	750	o	LYS A	97	26.857	77.959	-3.450	1.00	32.83
ATOM	751	N	LYS A	98	26.501	77.068	-2.683	1.00	34.44
ATOM	752	CA	LYS A	98	26.008	78.603	-4.243	1.00	26.62
ATOM	753	CB	LYS A	98	24.574	78.319	-4.215	1.00	22.39
ATOM	754	CG	LYS A	98	23.876	79.351	-3.319	1.00	23.74
ATOM	755	CD	LYS A	98	22.362	79.269	-3.276	1.00	22.19
ATOM	756	CE	LYS A	98	21.766	80.300	-2.335	1.00	22.81
ATOM	757	NZ	LYS A	98	20.251	80.160	-2.241	1.00	22.30
ATOM	758	C	LYS A	98	19.547	80.977	-3.253	1.00	21.47
ATOM	759	0	LYS A	98	23.990	78.346	-5.614	1.00	21.39
ATOM	760	N	ALA A	99	24.076	79.355	-6.301	1.00	23.12
ATOM	761	CA	ALA A	99	23.427	77.225	-6.044	1.00	21.69
ATOM	762	CB	ALA A	99	22.819	77.132	-7.369	1.00	23.49
ATOM	763	C	ALA A	99	23.126	75.756	-7.983	1.00	21.77
ATOM	764	0	ALA A	99	21.301	77.449	-7.439	1.00	22.78
ATOM	765	N	VAL A	100	20.834	78.065	-8.399	1.00	25.07
ATOM	766	CA	VAL A	100	20.547	77.040	-6.420	1.00	20.36
ATOM	767	CB	VAL A	100	19.106 18.462	77.274	-6.388	1.00	17.58
ATOM	768	CG1	VAL A	100	16.462	76.528	-5.196	1.00	16.99
ATOM	769	CG2			18.722	76.786	-5.130	1.00	14.03
ATOM	770	С			18.797	75.044	-5.313	1.00	15.21
ATOM	771	0			19.574	78.764	-6.277	1.00	20.86
ATOM	772	N			17.696	79.506	-5.697	1.00	25.82
ATOM	773	CA			17.236	79.201	-6.885	1.00	20.04
ATOM	774	CB			17.352	80.595	-6.829	1.00	17.64
ATOM	775	CG			18.682	81.316	-8.185	1.00	22.33
ATOM	776	CD			18.654	81.355	-8.862	1.00	27.61
ATOM	777	OE1			19.711	82.264	-10.048	1.00	28.27
ATOM	778	OE2			17.591	82.803	-10.393	1.00	35.84
ATOM	779	С			15.734	82.440 80.502	-10.656	1.00	33.44
ATOM	780	0			15.085		-6.561	1.00	18.04
ATOM	781	N			15.151	79.542 81.543	-6.977	1.00	20.27
ATOM	782	CA			13.727	81.512	-5.989	1.00	15.18
ATOM	783	CB			3.372	80.575	-5.749	1.00	14.63
ATOM	784	OG			4.095		-4.599	1.00	16.17
ATOM	785				.3.172	80.881 82.883	-3.441	1.00	19.01
ATOM	786	ο.			3.919	83.805	-5.512	1.00	14.90
ATOM	787	N			1.871	83.018	-5.226	1.00	16.69
ATOM	788	CA			1.135	84.261	-5.753	1.00	16.08
ATOM	789	CB	_		0.561		-5.579	1.00	14.05
ATOM	790				9.644	84.710 85.913	-6.928	1.00	11.82
ATOM	791				0.149	87.189	-6.849	1.00	14.83
ATOM	792				8.279	85.773	-6.601	1.00	16.95
ATOM	793				9.295	88.309	-7.081	1.00	11.21
ATOM	794				7.425	86.879	-6.583	1.00	12.90
ATOM	795				7.936	88.146	-7.065	1.00	10.94
ATOM	796	C I			0.004	83.930	-6.820	1.00	12.78
ATOM	797	0 1			9.249	82.981	-4.607	1.00	14.85
ATOM	798		CYS A 10		9.887	84.710	-4.822	1.00	14.06
ATOM	799	CA C	TYS A 10		3.853	84.484	-3.543 -2.548	1.00	14.45
							4.340	1.00	14.61

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		C D	CYS A 1	LO4	9.509	84.235	-1.194	1.00	14.79
MOTA	800 801	CB SG	÷ –		8.386	84.134	0.215	1.00	18.12
MOTA	802	C		104	7.896	85.662	-2.429	1.00	18.09
MOTA MOTA	803	ō		104	8.322	86.821	-2.482	1.00	18.91 17.06
ATOM	804	N		105	6.600	85.367	-2.339	1.00	13.87
ATOM	805	CA	TYR A	105	5.594	86.403	-2.161	1.00 1.00	12.35
ATOM	806	CB	TYR A	105	4.941	86.845	-3.486	1.00	14.43
ATOM	807	CG		105	4.103	85.830	-4.234 -4.110	1.00	9.55
ATOM	808	CD1		105	2.713	85.826	-4.832	1.00	7.61
MOTA	809	CEl		105	1.927	84.933 84.909	-5.112	1.00	11.05
MOTA	810	CD2		105	4.690 3.906	84.010	-5.846	1.00	13.52
MOTA	811	CE2		105	2.525	84.028	-5.699	1.00	15.44
ATOM	812	CZ		105 105	1.733	83.129	-6.395	1.00	18.33
MOTA	813	OH		105	4.576	85.967	-1.100	1.00	17.62
MOTA	814	C O		105	4.412	84.773	-0.820	1.00	14.49
ATOM	815 816	N		106	3.991	86.954	-0.432	1.00	18.67
MOTA	817	CA	LEU A	106	3.031	86.742	0.640	1.00	17.72
ATOM ATOM	818	CB	LEU A	106	3.437	87.602	1.844	1.00	15.11 18.61
ATOM	819	ÇG	LEU A	106	4.930	87.554	2.171 -	1.00	18.40
ATOM	820	CD1	LEU A	106	5.237	88.376	3.384	1.00 1.00	20.22
ATOM	821	CD2	LEU A	106	5.358	86.124	2.391 0.237	1.00	19.75
MOTA	822	С	LEU A	106	1.594	87.078	-0.947	1.00	19.55
MOTA	823	0	LEU A	106	1.266	87.191	1.253	1.00	19.69
MOTA	824	N	ASN A	107	0.753 -0.659	87.241 87.563	1.122	1.00	16.25
ATOM	825	CA	ASN A	107	-1.231	87.792	2.518	1.00	18.19
ATOM	826	CB	ASN A	107 107	-1.231	87.979	2.530	1.00	24.35
MOTA	827	CG	ASN A ASN A	107	-3.332	88.525	1.591	1.00	22.21
ATOM	828	OD1 ND2	ASN A	107	-3.362	87.551	3.618	1.00	16.86
MOTA	829	C ND2	ASN A	107	-0.817	88.812	0.279	1.00	15.33
ATOM	830 831	0	ASN A	107	-0.332	89.888	0.634	1.00	16.38
ATOM	832	N	PRO A	108	-1.497	88.686	-0.860	1.00	14.14 13.05
ATOM ATOM	833	CD	PRO A	108	-1.973	87.430	-1.466	1.00	14.52
ATOM	834	CA	PRO A	108	-1.712	89.818	-1.757	1.00	11.78
ATOM	835	СВ	PRO A	108	-2.552	89.206	-2.867	1.00	13.10
ATOM	836	CG	PRO A	108	-2.018	87.779	-2.916 -1.113	1.00	15.10
MOTA	837	С	PRO A	108	-2.409	91.006	-1.595	1.00	15.99
ATOM	838	0	PRO A	108	-2.295	92.126 90.776	-0.014	1.00	16.27
ATOM	839	N	ASN A	109	-3.114 -3.839	91.855	0.649	1.00	18.12
ATOM	840	CA	ASN A	109 109	-5.005	91.304	1.461	1.00	17.89
MOTA	841	CB	ASN A ASN A	109	-6.058	90.695	0.590	1.00	15.82
MOTA	842	CG OD1	ASN A	109	-6.374	91.228	-0.475	1.00	18.28
ATOM	843	ND2	ASN A	109	-6. 5 78	89.549	1.001	1.00	14.24
ATOM	844 845	C	ASN A	109	-2.990	92.759	1.511	1.00	19.06
ATOM	846	o	ASN A	109	-3.467	93.786	1.978	1.00	22.19 17.26
ATOM ATOM	847	N	PHE A	110	-1.762	92.349	1.791	1.00	13.51
ATOM	848	CA	PHE A	110	-0.879	93.168	2.588	1.00 1.00	11.28
ATOM	849	CB	PHE A	110	0.304	92.345	3.068	1.00	14.89
ATOM	850	CG	PHE A	110	-0.054	91.343	4.110 4.727	1.00	14.80
ATOM	851	CD1	PHE A	110	-1.296	91.384 90.365	4.494	1.00	16.71
MOTA	852	CD2	PHE A	110	0.854 -1.627	90.363	5.702	1.00	15.38
ATOM	853	CE1		110 110	0.532	89.440	5.474	1.00	14.69
MOTA	854	CE2	PHE A	110	-0.710	89.495	6.082	1.00	18.74
MOTA	855	CZ	PHE A	110	-0.404	94.363	1.787	1.00	16.88
MOTA	856	С 0	PHE A	110	0.469	94.243	0.930	1.00	21.88
MOTA	857 858	N	THR A	111	-1.032	95.509	2.004	1.00	18.68
ATOM	859	CA	THR A	111	-0.625	96.718	1.304	1.00	16.37 15.54
ATOM ATOM	860	CB	THR A	111	-1.764	97.305	0.482	1.00	18.30
ATOM	861	OG1	THR A	111	-2.723	97.911	1.355	1.00 1.00	11.84
ATOM	862	CG2	THR A	111	-2.423	96.221	-0.337	1.00	18.43
ATOM	863	С	THR A		-0.219	97.692	2.389 3.564	1.00	23.70
ATOM	864	0	THR A	_	-0.284	97.360	2.023	1.00	21.65
ATOM	865	N	PRO A		0.229	98.895	0.703	1.00	15.84
ATOM	866	CD	PRO A		0.707	99.351 99.845	3.069	1.00	23.93
MOTA	867	CA		_	0.626 1.273		2.272	1.00	21.58
MOTA	868	CB				_	1.079	1.00	19.10
MOTA	869	CG	PRO A				3.954	1.00	28.77
MOTA	870	C 0	PRO P		_		4.981	1.00	34.33
ATOM	871 872		ASP A		_		3.557	1.00	30.89
ATOM	6/2	••							

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ATOM	873	CA	ASP A	113	-2.908	100.608	4.325	1.00	29.23
ATOM	874	CB	ASP A	113	-4.095	100.876	3.403	1.00	33.62
ATOM ATOM	875	CG	ASP A	113	-3.740	101.759	2.229	1.00	39.32
ATOM	876 877	OD1		113	-3.551	102.980	2.420	1.00	38.82
ATOM	877	OD2		113	-3.659	101.220	1.107	1.00	41.64
ATOM	879	С 0	ASP A	113	-3.313	99.552	5.330	1.00	26.58
ATOM	880	И	ASP A HIS A	113	-4.020	99.831	6.288	1.00	30.47
ATOM	881	CA	HIS A	114	-2.875	98.327	5.090	1.00	22.11
ATOM	882	CB	HIS A	114 114	-3.203	97.223	5.964	1.00	18.51
ATOM	883	CG	HIS A	114	-2.562 -3.154	95.954	5.434	1.00	18.88
ATOM	884	CD2	HIS A	114	-3.955	94.695 93.771	5.980	1.00	20.47
ATOM	885	ND1	HIS A	114	-2.905	94.243	5.401 7.255	1.00	20.61
ATOM	886	CE1	HIS A	114	-3.527	93.092	7.440	1.00	21.89
ATOM	887	NE2	HIS A	114	-4.170	92.784	6.331	1.00 1.00	20.69
ATOM	888	C	HIS A	114	-2.682	97.529	7.347	1.00	16.26 20.91
ATOM	889	0	HIS A	114	-1.511	97.821	7.518	1.00	23.53
ATOM ATOM	890	N	PRO A	115	-3.535	97.414	8.365	1.00	23.07
ATOM	891 892	CD	PRO A	115	-4.933	96.973	8.311	1.00	24.88
ATOM	892 893	CA CB	PRO A	115	-3.148	97.688	9.745 -	1.00	24.93
ATOM	894	CG	PRO A PRO A	115	-4.411	97.334	10.525	1.00	27.48
ATOM	895	C	PRO A	115	-5.094	96.342	9.652	1.00	24.00
ATOM	896	o	PRO A	115 115	-1.927	96.923	10.233	1.00	26.06
ATOM	897	N	ARG A	116	-1.127 -1.782	97.456 95.678	10.991	1.00	32.32
ATOM	898	CA	ARG A	116	-0.634	94.868	9.802	1.00	26.43
ATOM	899	CB	ARG A	116	-0.810	93.430	10.199 9.727	1.00	26.26
ATOM	900	CG	ARG A	116	-1.813	92.629	10.516	1.00	30.69
ATOM	901	CD	ARG A	116	~1.372	92.533	11.950	1.00	35.60
ATOM	902	NE	ARG A	116	-2.151	91.547	12.685	1.00	39.57 44.77
ATOM	903	CZ	ARG A	116	-2.021	91.314	13.988	1.00	47.07
ATOM ATOM	904	NH1	ARG A	116	-1.145	91.997	14.721	1.00	44.22
ATOM	905	NH2	ARG A	116	-2.758	90.379	14.556	1.00	46.39
ATOM	906 907	C	ARG A	116	0.681	95.416	9.653	1.00	27.56
ATOM	908	O N	ARG A	116	1.727	95.273	10.276	1.00	28.41
ATOM	909	CA	ILE A ILE A	117 117	0.624	96.021	8.473	1.00	28.17
MOTA	910	CB	ILE A	117	1.806 1.584	96.580	7.835	1.00	28.31
ATOM	911	CG2	ILE A	117	2.790	96.734 97.357	6.307	1.00	24.00
ATOM	912	CG1	ILE A	117	1.315	95.372	5.644 5.668	1.00	23.25
ATOM	913	CD1	ILE A	117	2.506	94.482	5.596	1.00	20.98
ATOM	914	C	ILE A	117	2.140	97.930	8.490	1.00	16.97
ATOM	915	0	ILE A	117	3.308	98.237	8.742	1.00	34.06 40.01
ATOM	916	N	GLN A	118	1.111	98.716	8.797	1.00	34.32
ATOM ATOM	917	CA	GLN A	118	1.289	100.008	9.446	1.00	31.25
ATOM	918	CB	GLN A	118	-0.036	100.751	9.510	1.00	32.56
ATOM	919 920	CG CD	GLN A GLN A	118	-0.532	101.215	8.175	1.00	41.97
ATOM	921	OE1	GLN A	118	-1.790	102.040	8.289	1.00	49.04
ATOM	922	NE2	GLN A	118 118	-2.349 -2.241	102.203 102.577	9.374	1.00	54.55
ATOM	923	C	GLN A	118	1.813	99.816	7.167	1.00	54.77
ATOM	924	0	GLN A	118	2.606	100.602	10.857 11.348	1.00	30.00
ATOM	925	N	ALA A	119	1.362	98.759	11.506	1.00	36.36
ATOM	926	CA	ALA A	119	1.801	98.470	12.851	1.00	27.04
MOTA	927	CB	ALA A	11.9	0.898	97.447	13.457	1.00	23.94 23.97
ATOM	928	C	ALA A	119	3.223	97.944	12.836	1.00	29.31
ATOM	929	0	ALA A	119	3.839	97.802	13.885	1.00	35.94
ATOM ATOM	930	N		120	3.728	97.625	11.649	1.00	30.68
ATOM	931 932	CA CB		120	5.068	97.075	11.497	1.00	31.26
ATOM	933	CG		120	6.131	98.127	11.815	1.00	32.35
ATOM	934	CD		120 120	6.210	99.208	10.756	1.00	41.07
ATOM	935	CE		120	7.461 7.720	100.047	10.893	1.00	53.39
ATOM	936	NZ		120	9.046	100.864 101.563	9.621	1.00	60.71
ATOM	937	С		120	5.271	95.796	9.644	1.00	65.99
ATOM	938	0		120	6.266	95.633	12.321 13.014	1.00	30.21
ATOM	939	N		121	4.287	94.901	12.240	1.00	34.12
ATOM	940	CA		121	4.304	93.627	12.945	1.00 1.00	30.59
ATOM	941	CB	THR A	121	2.897	93.001	12.953	1.00	29.59
ATOM	942	OG1		121	1.948	93.993	13.347	1.00	26.01 29.93
ATOM	943	CG2		121	2.830	91.841	13.924	1.00	27.80
ATOM ATOM	944	C	THR A	21	5.238	92.685	12.203	1.00	31.22
ATOM	945	0	THR A	121	5.258	92.684	10.977	1.00	36.88

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							12.918	1.00	31.48
	946	N PR	O A 122	6.0		91.867	14.375	1.00	30.51
ATOM	947		O A 122	6.1		91.788	12.260	1.00	29.39
MOTA	948		O A 122			90.939	13.428	1.00	28.00
ATOM	949		RO A 122			90.162	14.508	1.00	28.89
MOTA	950		RO A 122			91.147	11.324	1.00	29.95
MOTA	951		RO A 122	6.2	213	89.993	11.499	1.00	33.22
MOTA	952		RO A 122	5.0	017	89.759	10.373	1.00	30.79
MOTA	953	-	HR A 123	6.5	957	89.422	9.355	1.00	28.32
ATOM	954		HR A 123	6.	470	88 472	9.961	1.00	30.03
ATOM	955		HR A 123	5.	859	87.189	10.661	1.00	35.13
ATOM	956		HR A 123	3 4.	648	87.498	10.897	1.00	31.48
MOTA	957	·	HR A 123	6.	835	86.507		1.00	27.79
MOTA			HR A 12	35.	505	89.028	8.309	1.00	29.06
ATOM	9 58 9 5 9	~	HR A 12	35.	164	88.310	7.377	1.00	24.80
MOTA	960		IS A 12	45.	076	90.285	8.458	1.00	22.12
MOTA		•	IS A 12	44.	150	90.920	7.504	1.00	17.07
MOTA	961		IS A 12	4 3.	072	91.740	8.226	1.00	13.05
MOTA	962		HIS A 12	4 2.	285	90.948	9.215	1.00	18.78
MOTA	963		HIS A 12	4 1.	.035	90.435	9.145	1.00	15.62
MOTA	964		HIS A 12		.798	90.529	10.420	1.00	17.88
MOTA	965		HIS A 12	4 1	.907	89.785	11.044	1.00	17.44
MOTA	966		HIS A 12	_	.825	89.712	10.292	1.00	21.71
MOTA	967		HIS A 12		.941	91.837	6.592	1.00	22.54
MOTA	968	_	HIS A 12	_	.645	92.715	7.050	1.00	21.78
MOTA	969	_			.819	91.632	5.295		20.92
ATOM	970	•-			.538	92.456	4.339	1.00	23.07
MOTA	971				.787	91.730	3.852	1.00	24.04
MOTA	972				.023	91.998	4.651	1.00	24.79
ATOM	973				.169	91.132	4.222	1.00	24.03
MOTA	974				.457	91.049	3.012	1.00	31.23
ATOM	975	OEl			.793	90.539	5.107	1.00	21.05
MOTA	976	OE2			1.668	92.738	3.143	1.00	24.62
MOTA	977	C			3.660	92.080	2.930	1.00	21.65
ATOM	978	0			5.091	93.694	2.339	1.00	
ATOM	979	И			4.361	94.031	1.146	1.00	22.78 20.08
MOTA	980	CA			4.203	95.538	1.042	1.00	
ATOM	981	CB			3.508	95.900	-0.229	1.00	17.38
ATOM	982	CG1			3.405	96.028	2.228	1.00	20.49
ATOM	983	CG2			5.166	93.459	-0.019	1.00	25.89
ATOM	984	С			6.380	93.667	-0.099	1.00	30.48
MOTA	985	0			4.511	92.683	-0.880	1.00	21.77
MOTA	986	N			5.174	92.053	-2.020	1.00	19.25
MOTA	987	CA		127	4.182	91.207	-2.830	1.00	18.25
MOTA	988	CB		127	3.724	89.985	-2.095	1.00	16.94
ATOM	989	CG		127	4.459	89.445	-1.286	1.00	16.08
MOTA	990	OD1	•	127	2.512	89.528	-2.380	1.00	12.62
ATOM	991	ND2		127	5.857	93.007	-2.975	1.00	19.23
MOTA	992	С	ASN A	127	5.436	94.150	-3.148	1.00	18.59
MOTA	993	0	ASN A	127	6.948	92.525	-3.556	1.00	18.95
ATOM	994	N	VAL A	128	7.698	93.260	-4.561	1.00	23.17
ATOM	995	CA	VAL A	128	9.228	93.403	-4.235	1.00	21.82
MOTA	996	CB	VAL A	128		94.284	-3.027	1.00	20.58
MOTA	997	CG1	VAL A	128	9.427 9.880	92.055	-3.999	1.00	23.71
MOTA	998	CG2	VAL A	128	7.494	92.408	-5.808	1.00	23.82
ATOM	999	С	VAL A	128		91.183	-5.730	1.00	23.35
ATOM	1000	0	VAL A	128	7.486	93.050	-6.951	1.00	25.96
ATOM	1001	N	TRP A	129	7.312	92.319	-8.179	1.00	28.04
ATOM	1002		TRP A	129	7.066	92.476	-8.562	1.00	22.71
MOTA	1003		TRP A	129	5.604	91.925	-7.588	1.00	20.42
ATOM	1004		TRP A	129	4.646	90.557	-7.467	1.00	17.81
	1005		TRP A	129	4.254		-6.508	1.00	16.80
ATOM	1006		TRP A	129	3.222	90.505	-8.084	1.00	17.14
MOTA	1007		TRP A	129	4.667		-6.710	1.00	15.97
MOTA	1008		TRP A	129	3.873		-6.063	1.00	17.97
MOTA	1000			129	3.008		-6.155	1.00	19.47
ATOM	101			129	2.597		-7.734	1.00	16.93
ATOM	101			129	4.048			1.00	
MOTA	101			129	3.024		0 336	1.00	03
MOTA	101	_	TRP A	129	7.887		2 225	1.00	
ATOM		_	TRP A	129	8.32			1.00	
MOTA	101		PRO A	130	8.10		40.400	1.00	
ATOM	101		PRO A		7.80			1.00	
MOTA	101		PRO A		8.88	0 92.47		1.00	
MOTA	101				9.10	9 91.19	2 -12.308	2.0	
MOTA	101		3						

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ATOM	1019	co	PRO	A 130	7.926	90 361			
ATOM	1020	С	PRO				,,,,	1.00	28.64
ATOM	1021	. 0	PRO			93.521		1.00	35.25
ATOM	1022	N	ASP			93.651	-12.146	1.00	36.95
ATOM	1023	CA				94.301	-13.100	1.00	38.98
ATOM	1024	CB		_		95.329	-13.927	1.00	41.94
ATOM	1025	CG		_	8.713	96.081	-14.699	1.00	49.89
MOTA	1026	OD			7.519	97.168	-15.612	1.00	59.35
ATOM	1027	OD				97.540	-15.503	1.00	60.33
ATOM	1028	С	ASP		9.499	97.667	-16.448	1.00	69.02
ATOM	1029	0	ASP		7.160	94.732	-14.895	1.00	40.13
ATOM	1030	N	GLU		7.444	93.761	-15.604	1.00	39.39
ATOM	1031	CA	GLU A		5.983	95.343	-14.933	1.00	38.57
ATOM	1032	CB	GLU A		4.895	94.906	-15.796	1.00	41.66
ATOM	1033	CG	GLU A		3.675	95.805	-15.594	1.00	49.43
ATOM	1034	CD	GLU A		2.565	95.210	-14.742	1.00	63.43
ATOM	1035	OE1			1.767	94.123	-15.455	1.00	68.77
ATOM	1036	OE2	•		1.390	93.130	-14.786	1.00	73.49
ATOM	1037	C			1.501	94.268	-16.671	1.00	70.44
ATOM	1038	0	GLU A		5.249	94.919	-17.269	1.00	
ATOM	1039		GLU A		4.925	93.984	-17.998	1.00	40.84
ATOM	1040	N	THR A		5.909	95.984	-17.709	1.00	42.27
ATOM		CA	THR A		6.261	96.124	-19.114	1.00	40.91
MOTA	1041	CB	THR A		7.100	97.407	-19.373		42.12
ATOM	1042	OG1			8.431	97.217	-18.884	1.00	43.93
ATOM	1043	CG2	THR A	133	6.496	98.602	-18.650	1.00	56.48
ATOM	1044	С	THR A	133	7.045	94.908	-19.576	1.00	42.47
ATOM	1045	0	THR A	133	6.800	94.369	-20.650	1.00	40.83
	1046	N	LYS A	134	7.945	94.450	-18.717	1.00	45.82
ATOM	1047	CA	LYS A	134	8.799	93.312	-19.014	1.00	40.62
ATOM	1048	CB	LYS A	134	10.109	93.429	-18.233	1.00	40.68
ATOM	1049	CG	LYS A	134	10.852	94.742	-18.437	1.00	44.31
ATOM	1050	CD	LYS A	134	12.171	94.754	-17.681	1.00	50.92
ATOM	1051	CE	LYS A	134	12.883	96.096	-17.881	1.00	56.36
A.TOM	1052	NZ	LYS A	134	14.159	96.104		1.00	64.21
ATOM	1053	C	LYS A	134	8.176	91.950	-17.026	1.00	72.09
MOTA	1054	0	LYS A	134	8.563	90.955	-18.737	1.00	40.31
ATOM	1055	N	HIS A	135	7.278	91.875	-19.348	1.00	45.00
ATOM	105€	CA	HIS A	135	6.649	90.601	-17.763	1.00	38.10
ATOM	1057	CB	HIS A	135	7.200	90.071	-17.425	1.00	34.82
ATOM	1058	CG	HIS A	135	8.654	89.705	-16.089	1.00	28.65
ATOM	1059	CD2	HIS A	135	9.267		-16.124	1.00	21.40
ATOM	1060	ND1	HIS A	135	9.659	88.523	-16.373	1.00	22.41
ATOM	1061	CE1	HIS A		10.832	90.614 90.012	-15.880	1.00	21.96
ATOM	1062	NE2	HIS A		10.624		-15.978	1.00	21.23
MOTA	1063	C	HIS A	135	5.135	88.743	-16.276	1.00	26.04
ATOM	1064	0	HIS A	135	4.536	90.787	-17.335	1.00	37.00
ATOM	1065	N	PRO A	136	4.489	90.584	-16.271	1.00	36.99
ATOM	1066	CD	PRO A	136	5.065	91.128	-18.465	1.00	38.00
ATOM	1067	CA	PRO A	136		91.093	-19.820	1.00	39.72
ATOM	1068	CB	PRO A	136	3.043	91.352	-18.545	1.00	35.57
ATOM	1069	CG	PRO A	136	2.801	91.478	-20.048	1.00	33.63
ATOM	1070	C	PRO A	136	3.882	90.651	-20.639	1.00	35.65
ATOM	1071	ō	PRO A	136	2.183	90.264	-17.935	1.00	33.54
ATOM	1072	N	GLY A		2.348	89.083	-18.231	1.00	35.53
ATOM	1073	CA	GLY A	137	1.284	90.680	-17.053	1.00	33.66
ATOM	1074	c	GLY A	137	0.379	89.753	-16.408	1.00 .	35.45
ATOM	1075	0	GLY A	137	0.946	88.810	-15.361	1.00	36.34
ATOM	1076	N		137	0.212	87.981	-14.829	1.00	41.58
ATOM	1077	CA	PHE A	138	2.224	88.926	-15.029	1.00	34.29
ATOM	1078		PHE A	138	2.792	88.034	-14.022	1.00	32.30
ATOM	1078	CB	PHE A	138	4.315	88.175	-13.960	1.00	
ATOM		CG	PHE A	138	4.960	87.272	-12.959	1.00	33.36
ATOM	1080	CD1	PHE A		4.770	85.902	-13.026	1.00	29.73
ATOM	1081	CD2	PHE A		5.718	87.796	-11.924	1.00	31.50
ATOM	1082	CE1	PHE A		5.322	85.061	-12.070	1.00	30.02
ATOM	1083	CE2	PHE A		6.272	B6.974	-10.965		32.69
	1084	CZ	PHE A	138	6.075	85.600	-11.035	1.00	30.29
ATOM	1085	C	PHE A	138	2.178	88.259	-12.639	1.00	33.63
ATOM	1086	0	PHE A		1.653	87.323	-12.029	1.00	31.05
ATOM	1087	N			2.205	89.502	-12.169	1.00	29.39
ATOM	1088	CA			1.662	89.816	-10.861	1.00	26.99
ATOM	1089	CB .	a		1.751	91.314	-10.581	1.00	28.51
ATOM	1090	CG			1.090	91.725	-9.275	1.00	23.97
ATOM	1091	CD			1.192	93.216	-8.982	1.00	27.92
					=		0.302	1.00	32.88

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ATOM 1093 NE2 GIN A 139 0.240 93.668 -7.987 1.00 31. ATOM 1094 NE2 GIN A 139 0.222 883.032 -10.734 1.00 31. ATOM 1095 O GIU A 139 0.126 88.663 -9.754 1.00 36. ATOM 1095 N ASP A 140 0.0.592 88.009 -11.752 1.00 35. ATOM 1096 N ASP A 140 0.0.592 88.009 -11.747 1.00 35. ATOM 1097 CB ASP A 140 0.2.716 88.766 1-12.972 1.00 40. ATOM 1098 CB ASP A 140 0.2.716 88.766 1-12.972 1.00 41. ATOM 1090 GD ASP A 140 0.1.391 91.955 12.266 1.00 57. ATOM 1100 GD ASP A 140 1.306 87.684 -11.694 1.00 49. ATOM 1101 OD ASP A 140 1.306 87.684 -11.694 1.00 49. ATOM 1102 C ASP A 140 1.1.906 91.840 -11.875 1.00 56. ATOM 1103 O ASP A 140 2.1.408 88.981 -11.694 1.00 34. ATOM 1105 CA PHE A 141 1.1.258 88.981 -12.396 1.00 35. ATOM 1106 CB PHE A 141 1.0.59 88.530 -12.373 1.00 32. ATOM 1106 CB PHE A 141 0.113 83.526 -13.1681 1.00 32. ATOM 1107 CC PHE A 141 0.113 83.526 -13.1681 1.00 32. ATOM 1109 CD2 PHE A 141 0.113 83.526 -13.1681 1.00 31. ATOM 1109 CD2 PHE A 141 0.013 82.456 -13.681 1.00 37. ATOM 1100 CD PHE A 141 0.013 82.456 -13.681 1.00 37. ATOM 1110 CD1 PHE A 141 0.013 83.536 -13.361 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 82.456 -13.364 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 82.456 -13.364 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 82.456 -13.364 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1111 CD2 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 -13.051 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM 1110 CD1 PHE A 141 0.073 81.149 1.00 37. ATOM	W () 30/100	40								
ATOM 1093 NEZ CIA A 139 - 0.212 09 31.668 - 7.997 1.00 31. ATOM 1094 C CIA A 139 - 0.125 09 311 10 0.33 1.00 13. ATOM 1095 C CIA A 139 - 0.125 09 5.69 - 11.752 1.00 13. ATOM 1096 C CIA A 139 - 0.125 09 5.69 - 11.752 1.00 13. ATOM 1097 CA ASP A 140 - 2.736 99.609 - 11.754 1.00 135 ATOM 1099 CC A ASP A 140 - 2.736 99.766 - 11.747 1.00 35 ATOM 1099 CC A ASP A 140 - 2.736 99.766 - 11.747 1.00 35 ATOM 1099 CC ASP A 140 - 2.736 99.766 - 11.747 1.00 49 ATOM 1099 CC ASP A 140 - 1.906 91.840 - 11.044 1.00 49 ATOM 1010 001 ASP A 140 - 1.906 91.840 - 11.044 1.00 49 ATOM 1010 002 ASP A 140 - 1.906 91.840 - 11.875 1.00 13. ATOM 1101 C C ASP A 140 - 1.906 91.840 - 11.875 1.00 13. ATOM 1104 N PME A 141 - 1.258 68 530 - 12.239 1.00 2.24 ATOM 1105 C A PHE A 141 - 1.259 68 530 - 12.179 1.00 2.24 ATOM 1106 CA PHE A 141 - 0.013 68 8.540 - 11.051 1.00 13. ATOM 1109 C C PHE A 141 - 0.013 68 530 - 12.368 1.00 13. ATOM 1109 C C PHE A 141 - 0.013 68 530 - 12.368 1.00 13. ATOM 1109 C C PHE A 141 - 0.113 68 530 - 12.368 1.00 13. ATOM 1109 C C PHE A 141 - 0.113 68 5.50 - 11.051 1.00 12. ATOM 1109 C C PHE A 141 - 0.013 68 5.50 - 12.368 1.00 13. ATOM 1109 C C PHE A 141 - 0.013 68 5.50 - 12.368 1.00 13. ATOM 1109 C C PHE A 141 - 0.013 68 5.50 - 12.368 1.00 13. ATOM 1110 C C PHE A 141 - 0.013 68 5.50 - 12.368 1.00 13. ATOM 1110 C C PHE A 141 - 0.013 68 5.60 - 13.364 1.00 13. ATOM 1111 C C PHE A 141 - 0.971 68 1.366 - 13.364 1.00 13. ATOM 1111 C C PHE A 141 - 0.971 68 1.366 - 13.364 1.00 13. ATOM 1112 C C PHE A 141 - 0.971 68 1.366 - 13.364 1.00 13. ATOM 1112 C C PHE A 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1112 C C PHE A 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1112 C C PHE A 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1112 C C PHE A 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1112 C C PHE A 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1112 C C PHE A 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1113 C C PHE A 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1114 O PHE G 141 - 0.971 68 1.366 - 13.369 1.00 13. ATOM 1114 O PHE G 141 - 0.9						- 57	•			
ATOM 1094 C GLN A 139 0.420 93.666 -7.997 1.00 42.70 ATOM 1095 C GLN A 139 0.222 89.693 -10.734 1.00 16.70 ATOM 1096 N ASP A 140 -0.592 89.695 -11.742 1.00 16.70 ATOM 1097 CA ASP A 140 -2.001 89.206 -11.742 1.00 16.70 ATOM 1098 CB ASP A 140 -2.001 89.206 -11.742 1.00 40.70 ATOM 1098 CB ASP A 140 -2.736 89.695 -11.872 1.00 10.70 ATOM 1099 CG ASP A 140 -2.736 89.695 -11.872 1.00 40.70 ATOM 1099 CG ASP A 140 -2.736 89.695 -11.872 1.00 55.70 ATOM 1099 CG ASP A 140 -2.736 89.70 1.00 1.00 1.00 ATOM 1090 CG ASP A 140 -2.736 89.10 1.00 1.00 1.00 ATOM 1090 CG ASP A 140 -2.100 89.609 -11.872 1.00 55.70 ATOM 1101 000 ASP A 140 -2.100 89.609 -11.875 1.00 55.70 ATOM 1101 000 ASP A 140 -2.100 89.609 -11.875 1.00 55.70 ATOM 1101 000 ASP A 140 -2.100 89.609 -11.895 1.10.00 55.70 ATOM 1101 000 ASP A 140 -2.100 89.609 -11.895 1.10.00 55.70 ATOM 1101 000 ASP A 140 -2.100 89.609 -11.694 1.00 34.70 ATOM 1101 000 ASP A 140 -1.2140 89.609 1.10.00 34.70 ATOM 1101 000 ASP A 140 -1.2140 89.609 1.10.00 34.70 ATOM 1101 000 ASP A 140 -1.2140 89.609 1.10.00 34.70 ATOM 1102 CB PHE A 141 -1.258 86.981 -12.389 1.00 229.70 ATOM 1108 CD PHE A 141 -1.258 86.981 -12.389 1.00 229.70 ATOM 1109 CD PHE A 141 -0.113 89.536 -13.3651 1.00 32.70 ATOM 1109 CD PHE A 141 -0.113 89.536 -13.3651 1.00 32.70 ATOM 1109 CD PHE A 141 -0.113 89.536 -13.3651 1.00 32.70 ATOM 1110 CC PHE A 141 -0.113 89.545 -13.3651 1.00 32.70 ATOM 1110 CC PHE A 141 -0.121 89.2651 -13.3651 1.00 32.70 ATOM 1111 CC PHE A 141 -0.121 89.2651 -13.3651 1.00 32.70 ATOM 1112 CC PHE A 141 -0.121 89.2651 -13.3651 1.00 32.70 ATOM 1112 CC PHE A 141 -0.121 89.2651 -13.3651 1.00 32.70 ATOM 1113 C PHE A 141 -0.121 89.60 AT	NEOM	1092	OE1	GLN A	139	1.943	93.950			32.97
ATOM 1095						0.440				31.33
ATOM 1096 M ASP A 140 -0.592 98.009 -11.792 1.00 15 ATOM 1097 CA ASP A 140 -0.592 98.009 -11.792 1.00 15 ATOM 1098 CB ASP A 140 -2.073 98.009 -11.792 1.00 40 ATOM 1098 CB ASP A 140 -2.073 98.076 -12.272 1.00 40 ATOM 1099 CG ASP A 140 -2.073 99.100 -12.026 1.00 40 ATOM 1100 CD ASP A 140 -1.091 91.895 -12.266 1.00 51 ATOM 1101 CD ASP A 140 -1.091 91.895 -12.266 1.00 51 ATOM 1102 CD ASP A 140 -1.091 87.684 -11.694 1.00 34 ATOM 1103 CD ASP A 140 -1.096 87.894 -11.603 1.00 35 ATOM 1104 N PHE A 141 -1.258 86.981 -12.189 1.00 34 ATOM 1105 CA PHE A 141 -1.258 86.981 -12.189 1.00 32 ATOM 1106 CB PHE A 141 -0.296 84.942 -13.168 1.00 32 ATOM 1107 CG PHE A 141 -0.193 85.530 -12.273 1.00 32 ATOM 1108 CD PHE A 141 -0.173 83.526 -13.051 1.00 33 ATOM 1109 CD PHE A 141 -0.173 83.266 -13.1681 1.00 33 ATOM 1109 CD PHE A 141 -0.173 83.266 -13.1681 1.00 33 ATOM 1110 CEI PHE A 141 -0.173 83.266 -13.1681 1.00 33 ATOM 1110 CEI PHE A 141 -0.971 80.266 -13.1688 1.00 33 ATOM 1111 CE PHE A 141 -0.971 80.266 -13.1688 1.00 33 ATOM 1111 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1111 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1111 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1111 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1111 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1111 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1111 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1112 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.791 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1113 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1114 CE PHE A 141 -0.971 80.056 -12.035 1.00 37 ATOM 1115 CE PHE A 141 -0.9			С	GLN A						33.84 36.68
ATOM 1096 N ASP A 140 -0.592 S3.005 -11.747		1095	0							37.09
ATOM 1098 CB ASP A 140 -2.736 99.776 -12.972 1.00 40 ATOM 1099 CG ASP A 140 -2.736 99.776 -12.972 1.00 40 ATOM 1009 CG ASP A 140 -2.736 99.1780 -13.041 1.00 40 ATOM 1100 OD1 ASP A 140 -1.996 91.890 -13.055 1.00 51 ATOM 1101 OD2 ASP A 140 -1.996 91.890 -13.055 1.00 51 ATOM 1101 CC ASP A 140 -1.996 97.890 -13.075 1.00 51 ATOM 1102 C ASP A 140 -1.996 87.149 -11.023 1.00 34 ATOM 1103 C ASP A 140 -1.996 87.149 -11.023 1.00 34 ATOM 1104 C B PHE A 141 -1.258 86.981 -12.389 1.00 29 ATOM 1105 C B PHE A 141 -1.258 86.981 -12.389 1.00 29 ATOM 1106 CB PHE A 141 -0.296 84.942 -13.368 1.00 26 ATOM 1107 C C PHE A 141 -0.721 82.456 -13.368 1.00 26 ATOM 1109 CD2 PHE A 141 -0.721 82.456 -13.364 1.00 37 ATOM 1109 CD2 PHE A 141 -0.373 81.143 -13.016 1.00 37 ATOM 1110 CE1 PHE A 141 -0.373 81.143 -13.016 1.00 37 ATOM 1110 CE2 PHE A 141 -0.973 81.93 -12.388 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.933 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1111 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1112 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1113 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1114 CZ PHE A 141 -0.821 85.033 1.0.969 1.00 37 ATOM 1115 NALA A 142 0.0567 85.093 1.0 4.99 1.00 37 ATOM 1116 CA ALA A 142 0.0567 85.093 1.0 4.99 1.00 32 ATOM 1117 CB ALA A 142 0.0567 85.093 1.0 4.99 1.00 32 ATOM 1119 O ALA A 142 0.0567 85.093 1.0 4.99 1.00 32 ATOM 1120 CG GUU A 143 1.169 86.477 1.00 32 ATOM 1121 CB GUI A 143 1.169 86.477 1.00 32 ATOM 1122 CB GUI A 143 1.169 86.477 1.00 32 ATOM 1123 CC GUI A 143 1.169 86.477 1.00 31 ATOM 1124 CC TYR A 144 -0.978 88.790 9.96 6.890 1.00 31 ATOM 1125 CB GUI A 143 1.169 88.790 9.96 9.96 6.890 1.00 31 ATOM 1126 CB GUI A 143 1.169 9.98 87.790 9.96 1.00		1096								35.96
ATOM 1099 CB APP A 140 - 2.672 91.000 -13.044 1.00 49 ATOM 11099 CD APP A 140 - 2.391 91.955 -12.266 1.00 56 ATOM 1100 OD1 ASP A 140 - 1.906 91.840 -13.875 1.00 56 ATOM 1102 OD ASP A 140 - 1.906 91.840 -13.875 1.00 56 ATOM 1102 O ASP A 140 - 3.024 87.149 -11.023 1.00 35 ATOM 1103 O APP A 140 - 3.024 87.149 -11.023 1.00 35 ATOM 1106 CD PHE A 141 - 1.258 86.981 -12.399 1.00 29 ATOM 1107 CG PHE A 141 - 1.258 86.981 -12.399 1.00 29 ATOM 1108 CD PHE A 141 - 0.296 84.942 -13.168 1.00 37 ATOM 1109 CD2 PHE A 141 - 0.296 84.942 -13.168 1.00 37 ATOM 1109 CD2 PHE A 141 - 0.296 84.942 -13.168 1.00 37 ATOM 1109 CD2 PHE A 141 - 0.297 82.456 -13.364 1.00 337 ATOM 1110 CD1 PHE A 141 - 0.298 84.942 -13.168 1.00 327 ATOM 1110 CD1 PHE A 141 - 0.973 81.143 -13.051 1.00 327 ATOM 1111 CD2 PHE A 141 - 0.973 81.143 -13.051 1.00 327 ATOM 1111 CD2 PHE A 141 - 0.973 81.143 -13.051 1.00 327 ATOM 1111 CD3 PHE A 141 - 0.973 81.143 -13.051 1.00 327 ATOM 1111 CD3 PHE A 141 - 0.973 81.143 -13.051 1.00 327 ATOM 1111 CD3 PHE A 141 - 0.973 81.143 -13.051 1.00 327 ATOM 1111 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1111 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1111 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1111 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1110 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1120 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1121 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1122 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1123 CD3 PHE A 141 - 0.973 81.143 -10.051 1.00 327 ATOM 1124 CD3 PHE A 142 - 0.973 81.143 81.454 -10.	MOTA									40.62
ATOM 1100 OD ASP A 140 -1-3.91 91.955 -12.266 1.00 51 ATOM 1101 OD ASP A 140 -1-3.90 91.800 -13.875 1.00 51 ATOM 1101 OD ASP A 140 -1-3.91 91.955 1.00 51 ATOM 1101 OD ASP A 140 -1-3.91 87.844 -11.694 1.00 34 ATOM 1103 O ASP A 140 -1-2.140 87.849 -11.003 1.00 34 ATOM 1103 N PHE A 141 -1.258 86.981 -12.389 1.00 34 ATOM 1105 C PHE A 141 -1.258 86.981 -12.389 1.00 29 ATOM 1106 CB PHE A 141 -1.305 85.530 -12.373 1.00 29 ATOM 1107 CG PHE A 141 -0.296 84.942 -13.368 1.00 26 ATOM 1108 CD1 PHE A 141 0.313 83.526 -13.051 1.00 32 ATOM 1109 CD2 PHE A 141 0.373 81.143 -13.016 1.00 37 ATOM 1110 CE1 PHE A 141 1.325 83.263 -12.388 1.00 37 ATOM 1110 CE2 PHE A 141 0.821 83.263 -12.388 1.00 37 ATOM 1111 CZ PHE A 141 0.821 83.263 -12.381 1.00 37 ATOM 1111 CZ PHE A 141 0.821 83.263 -12.381 1.00 37 ATOM 1110 CE2 PHE A 141 0.821 80.995 -12.149 1.00 31 ATOM 1111 CZ PHE A 141 0.821 85.033 10.996 12.00 31 ATOM 1111 CZ PHE A 141 0.821 85.033 10.996 12.00 31 ATOM 1116 CA ALA A 142 0.657 85.892 -8800 1.00 27 ATOM 1116 CA ALA A 142 0.657 85.932 -98.800 1.00 27 ATOM 1116 CA ALA A 142 0.657 85.932 -98.800 1.00 22 ATOM 1119 C ALA A 142 1.969 85.750 -6.970 1.00 23 ATOM 1120 CB ALA A 142 1.969 86.750 -6.970 1.00 24 ATOM 1121 CA CB ALA A 142 1.969 88.750 -6.970 1.00 24 ATOM 1122 CB CB ALA A 143 -1.262 89.916 -6.890 1.00 31 ATOM 1123 CB CB ALA A 143 -1.262 89.916 -6.890 1.00 31 ATOM 1124 CB CB CB ALA A 144 -0.996 91.448 -6.661 1.00 31 ATOM 1125 CB CB ALA A 144 -0.996 91.448 -6.651 1.00 31 ATOM 1126 CB CB ALA A 144 -0.997 88.750 -6.970 1.00 26 ATOM 1127 CB CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1128 CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1129 CB CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1120 CB CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1121 CB CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1123 CB CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1126 CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1127 CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1128 CB CB ALA A 144 -0.998 87.70 -6.990 1.00 31 ATOM 1129 CB										49.63
ATOM 1100 002 ASP A 140 -1.906 91.840 -11.694 1.00 56 ATOM 1102 C ASP A 140 -2.140 87.664 -11.694 1.00 34 ATOM 1103 C ASP A 140 -2.140 87.664 -11.694 1.00 34 ATOM 1104 N PHE A 141 -1.258 86.981 -12.389 1.00 35 ATOM 1105 CA PHE A 141 -1.258 86.981 -12.389 1.00 35 ATOM 1105 CA PHE A 141 -1.305 85.530 1.23.731 1.00 22 ATOM 1106 CB PHE A 141 -0.126 84.942 -13.368 1.00 36 ATOM 1107 CG PHE A 141 -0.126 84.942 -13.368 1.00 36 ATOM 1108 CD1 PHE A 141 -0.127 82.456 -13.3.651 1.00 37 ATOM 1109 CD2 PHE A 141 -0.127 83.263 -12.388 1.00 36 ATOM 1110 CE2 PHE A 141 -0.971 83.263 -12.388 1.00 37 ATOM 1111 CE2 PHE A 141 -0.971 83.263 -12.349 1.00 37 ATOM 1112 CZ PHE A 141 -0.971 85.033 -12.349 1.00 36 ATOM 1111 CP PHE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1111 CP PHE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1111 CP PHE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1111 CP PHE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1111 CP PHE A 141 -0.971 84.264 -10.369 1.00 32 ATOM 1111 CP PHE A 142 -0.971 85.033 -10.969 1.00 31 ATOM 1111 CP ALAA 142 0.162 85.493 -10.454 1.00 22 ATOM 1110 CP ALAA 142 0.162 85.493 -10.454 1.00 22 ATOM 1111 CP ALAA 142 -0.456 85.792 -8.880 1.00 32 ATOM 1110 CP ALAA 142 -0.438 84.480 -7.034 1.00 22 ATOM 1119 C ALAA 142 -0.438 84.480 -7.034 1.00 22 ATOM 1119 C ALAA 142 -0.438 84.480 -7.034 1.00 22 ATOM 112 CB GUD A 143 -1.969 86.750 -6.890 1.00 24 ATOM 112 CB GUD A 143 -1.969 86.750 -6.943 1.00 22 ATOM 112 CB GUD A 143 -1.969 86.750 -6.943 1.00 24 ATOM 112 CB GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 112 CB GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 113 CG GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 113 CB GUD A 143 -1.262 89.168 -6.691 1.00 32 ATOM 112 CB GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 113 CB GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 113 CB GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 113 CB GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 1140 CB TYR A 145 -0.991 88.199 91.00 31 ATOM 1140 CD TYR A 145 -0.991 88.339 -7.933 1.00 32 ATOM 113 CB GUD A 143 -1.262 89.168 -6.681 1.00 32 ATOM 113 CB GUD A 14									1.00	51.54
AROM 1102 C ASP A 140 -2.1400 87.694 -11.694 1.00 34 AROM 1103 O ASP A 140 -1.024 87.149 -11.023 1.00 35 AROM 1104 N PHE A 141 -1.258 86.981 -12.389 1.00 29 AROM 1105 CA PHE A 141 -1.258 86.981 -12.389 1.00 29 AROM 1106 CB PHE A 141 -0.296 86.981 -12.389 1.00 39 AROM 1106 CB PHE A 141 -0.296 84.942 -13.3.681 1.00 36 AROM 1107 CC PHE A 141 -0.296 84.942 -13.3.681 1.00 36 AROM 1108 CD1 PHE A 141 -0.226 84.942 -13.3.681 1.00 36 AROM 1109 CD2 PHE A 141 -0.721 82.456 -13.3.681 1.00 36 AROM 1109 CD2 PHE A 141 -0.721 82.456 -13.3.681 1.00 36 AROM 1110 CE1 PHE A 141 -0.721 83.263 -12.389 1.00 36 AROM 1111 CC2 PHE A 141 -0.373 81.143 -13.016 1.00 36 AROM 1111 CC2 PHE A 141 -0.373 81.143 -13.016 1.00 36 AROM 1112 CC2 PHE A 141 -0.821 80.885 -12.0359 1.00 36 AROM 1113 C PHE A 141 -0.271 85.033 -10.369 1.00 36 AROM 1114 O PHE A 141 -0.721 85.033 -10.369 1.00 36 AROM 1114 O PHE A 141 -0.721 85.033 -10.369 1.00 36 AROM 1115 N ALAA 142 0.627 86.933 -10.454 1.00 37 AROM 1116 CA ALAA 142 0.627 86.933 -10.454 1.00 23 AROM 1116 CA ALAA 142 0.627 86.933 -10.454 1.00 23 AROM 1116 CA ALAA 142 0.047 88 84.480 -7.094 1.00 23 AROM 1117 CB ALAA 142 -0.438 84.480 -7.094 1.00 23 AROM 1119 O ALAA 142 -0.438 84.480 -7.094 1.00 23 AROM 1112 CG GLU A 143 -1.999 86.750 -6.970 1.00 24 AROM 1122 CG GLU A 143 -1.999 86.750 -6.970 1.00 24 AROM 1122 CG GLU A 143 -1.999 86.750 -6.970 1.00 24 AROM 1122 CG GLU A 143 -1.999 86.750 -6.970 1.00 27 AROM 1122 CG GLU A 143 -1.999 86.750 -6.970 1.00 27 AROM 1123 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1124 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1125 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1127 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1127 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1128 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1126 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1127 CG GLU A 143 -1.999 86.750 -6.970 1.00 37 AROM 1126 CG GLU A 143 -1.990 86.750 -6.970 1.00 37 AROM 1127 CG GLU A 143 -1.900 89.910 -6.991 1.00 37 AROM 1126 CG GLU A 143 -9.906 91.448 -7.918 1.								-13.875	1.00	56.38
ATOM 1104 N PHE A 141 -1.258 86.981 -12.389 1.00 29 ATOM 1105 CA PHE A 141 -1.258 86.981 -12.389 1.00 29 ATOM 1105 CA PHE A 141 -1.258 86.981 -12.389 1.00 29 ATOM 1106 CB PHE A 141 -1.305 85.530 1.23.373 1.00 29 ATOM 1106 CB PHE A 141 0.113 85.530 1.3.051 1.00 32 ATOM 1107 CG PHE A 141 0.113 83.526 1.33.051 1.00 33 ATOM 1108 CD1 PHE A 141 0.113 83.526 -13.3.051 1.00 33 ATOM 1109 CD2 PHE A 141 0.113 83.526 -13.3.051 1.00 33 ATOM 1109 CD2 PHE A 141 1.312 83.263 -12.388 1.00 33 ATOM 1110 CD2 PHE A 141 1.512 83.263 -12.388 1.00 33 ATOM 1111 CD2 PHE A 141 0.571 83.263 -12.389 1.00 33 ATOM 1111 CD2 PHE A 141 0.671 85.033 -12.0359 1.00 33 ATOM 1112 CZ PHE A 141 0.671 85.033 -12.0359 1.00 31 ATOM 1113 CD PHE A 141 -0.571 85.033 -10.969 1.00 31 ATOM 1114 CD PHE A 141 -0.571 85.033 -10.969 1.00 31 ATOM 1115 N ALA A 142 0.162 85.493 -10.464 1.00 2.27 ATOM 1116 CA ALA A 142 0.167 85.493 -10.464 1.00 2.27 ATOM 1119 C ALA A 142 0.167 85.493 -0.498 1.00 2.27 ATOM 1119 C ALA A 142 0.167 85.493 -0.498 1.00 2.27 ATOM 1119 C ALA A 142 0.167 85.791 -0.994 1.00 2.27 ATOM 1119 C ALA A 142 0.187 85.791 -0.994 1.00 2.27 ATOM 1119 C ALA A 142 0.187 85.791 -0.994 1.00 2.27 ATOM 1120 N GUD A 143 -1.059 86.470 -7.995 1.00 2.27 ATOM 1120 CB GUD A 143 -1.969 86.470 -7.995 1.00 2.27 ATOM 1120 CB GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1121 CG GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1122 CB GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1123 CG GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1124 CD GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1127 CG GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1127 CG GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1129 CD GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1129 CG GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1124 CD GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1124 CD GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1124 CD GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1124 CD GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1124 CD GUD A 143 -1.762 88.211 -7.077 1.00 2.27 ATOM 1124 CD GUD							87.684			34.15
ATOM 1104 N PHE A 141 -1.258 86.981 -12.373 1.00 29 ATOM 1106 CB PHE A 141 -0.296 85.530 -12.373 1.00 29 ATOM 1106 CB PHE A 141 -0.296 84.942 1.33.368 1.00 36 ATOM 1108 CD1 PHE A 141 -0.721 82.456 -13.3.681 1.00 37 ATOM 1109 CD2 PHE A 141 -0.721 82.456 -13.3.681 1.00 37 ATOM 1109 CD2 PHE A 141 -0.721 82.456 -13.3.681 1.00 37 ATOM 1109 CD2 PHE A 141 -0.373 81.143 1.1.016 1.00 37 ATOM 1110 CD1 PHE A 141 -0.373 81.143 1.1.016 1.00 37 ATOM 1111 CD2 PHE A 141 -0.373 81.143 1.1.016 1.00 37 ATOM 1112 CZ PHE A 141 -0.371 85.033 -10.969 1.00 37 ATOM 1114 O PHE A 141 -0.791 85.033 -10.969 1.00 37 ATOM 1115 N ALA A 142 -0.162 85.493 -10.454 1.00 27 ATOM 1116 CA ALA A 142 -0.657 85.091 -10.454 1.00 27 ATOM 1116 CA ALA A 142 -0.371 85.033 -10.969 1.00 37 ATOM 1117 CB ALA A 142 -0.371 85.033 -10.969 1.00 37 ATOM 1118 C ALA A 142 -0.377 85.031 -10.454 1.00 22 ATOM 1119 O ALA A 142 -0.317 85.031 -10.7995 1.00 22 ATOM 1119 O ALA A 142 -0.317 85.031 -10.7995 1.00 22 ATOM 1119 C ALA A 142 -0.317 85.031 -10.454 1.00 22 ATOM 1119 O ALA A 142 -0.317 85.313 -10.999 1.00 32 ATOM 1120 N GUD A 143 -1.033 86.437 -8.032 1.00 32 ATOM 1120 CG GUD A 143 -1.033 86.437 -8.032 1.00 32 ATOM 1121 CG GUD A 143 -1.033 86.437 -8.032 1.00 32 ATOM 1122 CG GUD A 143 -1.033 86.437 -8.032 1.00 32 ATOM 1124 CD GUD A 143 -1.969 86.750 -6.570 1.00 22 ATOM 1125 OEI GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1126 OEZ GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1127 C GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1128 OE GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1129 N GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1126 OEZ GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1127 C GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1128 OE GUD A 143 -1.733 90.618 -6.881 1.00 34 ATOM 1129 N GUD A 144 -1.734 84.284 94.98 94.99 94.99 94.99 94.99 94.90 94.9					140	-3.024				35.48
ATOM 1106 CA PHE A 141 -1.305 85.530 1.20.31.68 1.00 326 ATOM 1107 CG PHE A 141 0.113 33.526 1.30.51 1.00 326 ATOM 1108 CD1 PHE A 141 0.113 33.526 1.30.51 1.00 327 ATOM 1109 CD2 PHE A 141 1.312 83.526 1.33.051 1.00 337 ATOM 1109 CD2 PHE A 141 1.312 83.263 1.23.388 1.00 35 ATOM 1110 CD2 PHE A 141 1.312 83.263 1.23.388 1.00 35 ATOM 1111 CD2 PHE A 141 1.667 81.956 1.20.35 1.00 37 ATOM 1111 CD2 PHE A 141 1.667 81.956 1.20.35 1.00 37 ATOM 1111 CD2 PHE A 141 1.667 81.956 1.20.35 1.00 37 ATOM 1112 CZ PHE A 141 0.621 80.895 1.20.349 1.00 35 ATOM 1113 C PHE A 141 1.677 81.956 1.20.35 1.00 37 ATOM 1115 CA ALA A 142 0.162 85.493 1.00.969 1.00 34 ATOM 1116 CA ALA A 142 0.162 85.493 1.00.454 1.00 223 ATOM 1117 CB ALA A 142 0.162 85.493 1.00.454 1.00 233 ATOM 1119 C ALA A 142 0.057 85.091 9.149 1.00 233 ATOM 1119 C ALA A 142 0.488 84.480 7.094 1.00 233 ATOM 1119 O ALA A 142 0.488 84.480 7.094 1.00 233 ATOM 1112 CA GLU A 143 1.1969 86.750 -6.970 1.00 34 ATOM 1121 CA GLU A 143 1.1969 86.750 -6.970 1.00 324 ATOM 1121 CA GLU A 143 1.1969 86.750 -6.970 1.00 324 ATOM 1121 CA GLU A 143 1.1969 86.750 -6.970 1.00 324 ATOM 1121 CA GLU A 143 1.1969 86.750 -6.970 1.00 324 ATOM 1122 CG GLU A 143 -1.969 81.760 86.750 -6.970 1.00 324 ATOM 1121 CA GLU A 143 -1.262 89.196 -6.993 1.00 31 ATOM 1122 CG GLU A 143 -1.262 89.196 -6.993 1.00 31 ATOM 1124 CD GLU A 143 -1.262 89.196 -6.993 1.00 31 ATOM 1125 OEI GLU A 143 -1.262 89.196 -6.993 1.00 31 ATOM 1126 OEI GLU A 143 -1.262 89.196 -6.993 1.00 31 ATOM 1127 C GLU A 143 -1.262 89.196 -7.999 1.00 34 ATOM 1128 O GLU A 143 -1.313 95.618 -6.681 1.00 31 ATOM 1129 N GLU A 143 -1.313 95.618 -6.891 1.00 31 ATOM 1126 OEI GLU A 143 -1.313 90.618 -6.891 1.00 31 ATOM 1127 C GLU A 143 -1.262 89.196 -6.993 1.00 31 ATOM 1128 O GLU A 143 -1.313 90.618 -6.891 1.00 31 ATOM 1126 OEI GLU A 143 -1.313 90.618 -6.891 1.00 31 ATOM 1126 OEI GLU A 143 -1.313 90.618 -6.891 1.00 31 ATOM 1126 OEI GLU A 143 -1.313 90.618 -6.891 1.00 31 ATOM 1126 OEI GLU A 144 -1.313 90.618 -6.891 1.00 31 ATOM 1127 C GLU A 144 -1.313 90.618 -6.					141	-1.258				29.30 29.22
ATOM 1106 CB PHE A 141 -0.296 94.942 1.1.105 1.00 37 ATOM 1108 CD1 PHE A 141 -0.721 82.456 -11.1561 1.00 37 ATOM 1109 CD2 PHE A 141 -0.721 82.456 -11.1561 1.00 37 ATOM 1100 CD2 PHE A 141 -0.721 82.456 -11.1561 1.00 37 ATOM 1110 CD2 PHE A 141 -0.373 81.143 -11.046 1.00 37 ATOM 1110 CD2 PHE A 141 -0.373 81.143 -11.046 1.00 37 ATOM 1111 CD2 PHE A 141 -0.373 81.143 -11.046 1.00 37 ATOM 1111 CD2 PHE A 141 -0.373 81.143 -11.046 1.00 37 ATOM 1111 CD2 PHE A 141 -0.371 85.033 -10.969 1.00 31 ATOM 1113 CD PHE A 141 -0.371 85.033 -10.969 1.00 31 ATOM 1114 CD PHE A 141 -1.720 84.264 -10.169 1.00 34 ATOM 1115 N ALA A 142 0.657 85.093 -10.454 1.00 32 ATOM 1116 CA ALA A 142 0.657 85.093 -0.949 1.00 32 ATOM 1116 CA ALA A 142 0.657 85.093 -0.949 1.00 32 ATOM 1118 C ALA A 142 -0.317 85.313 -10.454 1.00 32 ATOM 1118 C ALA A 142 -0.317 85.313 -7.995 1.00 32 ATOM 1119 O ALA A 142 -0.418 84.480 -7.994 1.00 32 ATOM 1120 N GUU A 143 -1.039 88.437 -8.022 1.00 32 ATOM 1120 N GUU A 143 -1.039 88.437 -8.022 1.00 32 ATOM 1121 CA GUU A 143 -1.039 88.437 -8.022 1.00 32 ATOM 1122 CB GUU A 143 -1.799 86.750 -8.970 1.00 32 ATOM 1124 CD GUU A 143 -1.739 90.618 -6.6970 1.00 32 ATOM 1125 CB GUU A 143 -1.739 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.739 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1127 C GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1127 C GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1127 C GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1127 C GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1127 C GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1130 CB GUU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 11			CA	PHE A	141					26.63
ATOM 1106 CD PRE A 141 0.143 83.263 -12.364 1.00 37 ATOM 1108 CD1 PRE A 141 1.312 83.263 -12.388 1.00 36 ATOM 1108 CD2 PRE A 141 1.312 83.263 -12.388 1.00 36 ATOM 1110 CE1 PRE A 141 1.373 81.141 -13.016 1.00 37 ATOM 1111 CE2 PRE A 141 1.667 81.965 -12.389 1.00 37 ATOM 1111 CE2 PRE A 141 1.667 81.965 -12.349 1.00 37 ATOM 1112 CZ PRE A 141 0.821 80.855 -12.349 1.00 37 ATOM 1113 C PRE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1113 C PRE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1115 N ALA A 142 0.162 85.493 -10.464 1.00 27 ATOM 1115 N ALA A 142 0.162 85.493 -10.464 1.00 27 ATOM 1116 CA ALA A 142 1.969 85.792 -0.889 1.00 32 ATOM 1117 CB ALA A 142 1.969 85.792 -0.889 1.00 32 ATOM 1119 O ALA A 142 -0.438 84.480 -7.098 1.00 32 ATOM 1119 O ALA A 142 -0.438 84.480 -7.094 1.00 22 ATOM 1120 N GUU A 143 -1.013 86.437 -8.090 1.00 32 ATOM 1121 CA GUU A 143 -1.013 86.437 -8.090 1.00 32 ATOM 1122 CB GUU A 143 -1.969 86.750 -6.970 1.00 32 ATOM 1122 CB GUU A 143 -1.769 86.750 -6.970 1.00 32 ATOM 1124 CD GUU A 143 -1.769 86.750 -6.970 1.00 32 ATOM 1125 CB GUU A 143 -1.262 89.196 -6.890 1.00 31 ATOM 1126 CB GUU A 143 -1.669 91.448 -6.250 1.00 31 ATOM 1127 C GUU A 143 -1.383 85.824 -7.018 1.00 31 ATOM 1127 C GUU A 143 -3.183 85.824 -7.018 1.00 31 ATOM 1128 O GUU A 143 -3.183 85.824 -7.018 1.00 31 ATOM 1129 N GUN A 144 -3.699 85.596 -8.219 1.00 31 ATOM 1130 CB GUN A 144 -3.699 85.596 -8.219 1.00 31 ATOM 1130 CB GUN A 144 -3.699 85.596 -8.219 1.00 31 ATOM 1130 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -7.754 84.269 -9.309 1.00 31 ATOM 1131 CB GUN A 144 -		1106	CB							32.93
ATOM 1108 CD1 PRE A 141 -0.721 82.403 -12.388 1.00 37 ATOM 1110 CD1 PRE A 141 -0.373 81.143 -13.016 1.00 37 ATOM 1110 CD1 PRE A 141 -0.373 81.143 -13.016 1.00 37 ATOM 1111 CD2 PRE A 141 -0.373 81.143 -13.016 1.00 37 ATOM 1111 CD2 PRE A 141 -0.371 85.033 -10.969 1.00 38 ATOM 1112 CD PRE A 141 -0.971 85.033 -10.969 1.00 38 ATOM 1113 C PRE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1115 N ALA A 142 0.667 85.033 -10.969 1.00 31 ATOM 1116 CA ALA A 142 0.667 85.093 -10.454 1.00 27 ATOM 1116 CA ALA A 142 0.667 85.093 -10.454 1.00 27 ATOM 1116 CA ALA A 142 0.667 85.093 -19.149 1.00 27 ATOM 1117 CB ALA A 142 0.489 85.792 -8.880 1.00 26 ATOM 1117 CB ALA A 142 -0.317 85.313 -7.995 1.00 22 ATOM 1119 O ALA A 142 -0.317 85.313 -7.995 1.00 22 ATOM 1119 O ALA A 142 -0.438 84.480 -7.094 1.00 27 ATOM 1120 N GLU A 143 -1.013 86.437 -8.022 1.00 24 ATOM 1121 CA GLU A 143 -1.013 86.437 -8.022 1.00 24 ATOM 1122 CB GLU A 143 -1.026 88.8916 6.890 1.00 31 ATOM 1122 CB GLU A 143 -1.026 88.9196 6.890 1.00 31 ATOM 1124 CD GLU A 143 -1.733 90.618 -6.691 1.00 32 ATOM 1126 ODE GLU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1126 ODE GLU A 143 -1.733 90.618 -6.691 1.00 34 ATOM 1127 C GLU A 143 -3.640 85.318 -5.989 1.00 34 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 34 ATOM 1128 O GLU A 143 -3.690 85.596 -8.219 1.00 34 ATOM 1128 O GLU A 143 -3.690 85.596 -8.219 1.00 34 ATOM 1127 C GLU A 144 -3.833 84.725 -8.392 1.00 34 ATOM 1130 CB GLU A 144 -5.292 83.852 -10.139 1.00 34 ATOM 1131 CB GLU A 144 -5.278 84.696 -9.858 1.00 3 ATOM 1131 CB GLU A 144 -5.279 83.852 -10.139 1.00 3 ATOM 1131 CB GLU A 144 -5.279 83.852 -10.139 1.00 3 ATOM 1131 CB GLU A 144 -5.279 83.852 -10.139 1.00 5 ATOM 1131 CB GLU A 144 -5.279 83.852 -10.139 1.00 5 ATOM 1131 CB GLU A 144 -5.279 83.852 -10.139 1.00 5 ATOM 1131 CB GLU A 144 -5.201 82.669 -7.938 1.00 3 ATOM 1131 CB GLU A 144 -5.201 82.669 -7.938 1.00 3 ATOM 1131 CB GLU A 144 -5.201 82.669 -7.938 1.00 3 ATOM 1131 CB GLU A 144 -5.201 82.669 -7.939 1.00 3 ATOM 1131 CB GLU A 144 -5.201 82.669 -7.939 1.00 3 ATOM 1131 CB GLU A 1	ATOM	1107								37.47
ATOM 1100 CD2 PHE A 141 -0.373 B1.143 -13.016 1.00 37 ATOM 1111 CE2 PHE A 141 -0.373 B1.56 -12.055 1.00 37 ATOM 1111 CE2 PHE A 141 1.667 B1.065 -12.055 1.00 37 ATOM 1112 CZ PHE A 141 0.621 80.895 -12.349 1.00 31 ATOM 1113 C PHE A 141 -0.971 B5.033 -10.969 1.00 31 ATOM 1114 O PHE A 141 -1.720 84.264 -10.369 1.00 32 ATOM 1115 N ALA A 142 0.162 B5.493 -10.454 1.00 22 ATOM 1115 CA ALA A 142 0.167 B5.091 9.149 1.00 22 ATOM 1116 CA ALA A 142 1.969 B5.792 -8.880 1.00 24 ATOM 1119 O ALA A 142 1.969 B5.792 -8.880 1.00 24 ATOM 1119 O ALA A 142 -0.438 B4.480 -7.094 1.00 23 ATOM 1119 O ALA A 142 -0.438 B4.480 -7.094 1.00 23 ATOM 1120 CA GLU A 143 -1.033 B6.437 -8.022 1.00 24 ATOM 1121 CA GLU A 143 -1.969 B6.750 -6.970 1.00 24 ATOM 1122 CB GLU A 143 -1.969 B6.750 -6.970 1.00 24 ATOM 1123 CG GLU A 143 -1.262 B9.196 -6.890 1.00 31 ATOM 1124 CD GLU A 143 -1.733 90.618 6.681 1.00 31 ATOM 1125 OEE GLU A 143 -1.262 B9.196 -6.890 1.00 31 ATOM 1126 OEE GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1127 C GLU A 143 -1.91 9.906 91.448 -6.250 1.00 44 ATOM 1128 OEL GLU A 143 -1.93 90.966 91.448 -6.250 1.00 44 ATOM 1127 C GLU A 143 -3.690 B5.596 -8.219 1.00 34 ATOM 1126 OEE GLU A 143 -3.690 B5.596 -8.219 1.00 34 ATOM 1127 C GLU A 143 -3.690 B5.596 -8.219 1.00 34 ATOM 1130 CA GLU A 144 -3.699 B5.596 -8.219 1.00 34 ATOM 1130 CA GLU A 144 -3.699 B5.596 -9.858 1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 -9.858 1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 -9.858 1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 -9.858 1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 -9.858 1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 -9.858 1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 -9.858 1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 B5.596 B5.599 B1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 B5.596 B5.599 B1.00 34 ATOM 1131 CG GLU A 144 -3.699 B5.596 B5.596 B5.599 B1.00 34 ATOM 1131 CG GLU A 144 -4.494 B5.329 B5.596 B5.596 B5.599 B1.00 34 ATOM 1131 CG GLU A 144 -4.494 B5.329 B5.596 B5.595 B5.596 B5.599 B1.00 34 ATOM 1131 CG GLU A 144 -4.494 B5.329 B5.596 B5.595 B5.	ATOM									36.97
ATOM 1110 CEL PRE A 141 1 .667 81.956 -12.035 1.00 37 ATOM 1112 CZ PRE A 141 0.821 80.895 -12.149 1.00 36 ATOM 1112 CZ PRE A 141 0.821 80.895 -12.149 1.00 36 ATOM 1113 C PRE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1114 0 PRE A 141 -1.720 84.264 -10.369 1.00 31 ATOM 1115 N ALA A 142 0.662 85.493 -10.454 1.00 23 ATOM 1116 CA ALA A 142 0.667 85.091 -9 149 1.00 23 ATOM 1116 CA ALA A 142 0.657 85.091 -9 149 1.00 23 ATOM 1117 CE ALA A 142 1.969 85.792 -8 8.800 1.00 24 ATOM 1118 C ALA A 142 -0.117 85.313 -7 .995 1.00 23 ATOM 1118 C ALA A 142 -0.117 85.313 -7 .995 1.00 23 ATOM 1119 O ALA A 142 -0.438 84.480 -7 .094 1.00 23 ATOM 1120 N GLU A 143 -1.013 86.437 -8 .022 1.00 24 ATOM 1121 CA GLU A 143 -1.059 85.750 -6.970 1.00 24 ATOM 1122 CE GLU A 143 -2.403 88.211 -7 .077 1.00 22 ATOM 1122 CE GLU A 143 -1.726 89.196 -6.890 1.00 31 ATOM 1125 CEI GLU A 143 -1.733 90.618 -6.681 1.00 31 ATOM 1126 CEI GLU A 143 -1.733 90.618 -6.681 1.00 31 ATOM 1126 CEI GLU A 143 -1.733 90.618 -6.681 1.00 31 ATOM 1127 C GLU A 143 -3.640 85.318 -5.989 1.00 31 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 31 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 31 ATOM 1129 N GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1129 N GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1130 CA GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CE GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CE GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CE GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CE GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CE GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CE GLU A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CE GLU A 144 -4.849 83.339 -7.938 1.00 2 ATOM 1133 CE GLU A 144 -4.849 83.339 -7.938 1.00 34 ATOM 1134 CE TYR A 145 -0.855 79.959 1.00 34 ATOM 1134 CE TYR A 145 -0.855 79.959 1.00 34 ATOM 1134 CE TYR A 145 -0.855 79.959 1.00 34 ATOM 1134 CE TYR A 145 -0.855 79.959 1.00 34 ATOM 1135 CE TYR A 145 -0.855 79.959 1.00 34 ATOM 1135 CE TYR A 145 -0.855 79.959 1.00 34 ATOM 1135 CE TYR A 145 -0.855 79.959 1.00 34 ATOM 1135 CE TYR										37.55
ATOM 1112 CZ PHE A 141 0.821 80.895 -12.349 1.00 36 ATOM 1113 C PHE A 141 -0.971 83.033 -10.969 1.00 31 ATOM 1115 N ALA A 142 0.152 85.033 -10.969 1.00 34 ATOM 1115 N ALA A 142 0.657 85.091 -0.454 1.00 23 ATOM 1116 CA ALA A 142 0.657 85.091 -9.149 1.00 23 ATOM 1117 CB ALA A 142 1.969 85.792 -8.880 1.00 23 ATOM 1119 C ALA A 142 -0.458 84.480 -7.094 1.00 23 ATOM 1119 O ALA A 142 -0.438 84.480 -7.094 1.00 23 ATOM 1120 N GLU A 143 -1.969 86.750 -6.970 1.00 24 ATOM 1121 CA GLU A 143 -1.969 86.750 -6.870 1.00 24 ATOM 1122 CG GLU A 143 -1.262 89.196 -6.890 1.00 24 ATOM 1123 CG GLU A 143 -1.262 89.196 -6.890 1.00 36 ATOM 1124 CD GLU A 143 -1.262 89.196 -6.890 1.00 36 ATOM 1125 OEI GLU A 143 -0.906 91.448 -6.250 1.00 36 ATOM 1126 OEZ GLU A 143 -3.183 85.824 -7.018 1.00 24 ATOM 1127 C GLU A 143 -1.999 85.596 -6.890 1.00 36 ATOM 1128 O GLU A 143 -1.313 85.824 -7.018 1.00 24 ATOM 1126 OEZ GLU A 143 -1.699 81.596 -6.891 1.00 36 ATOM 1127 C GLU A 143 -1.89 85.591 9.916 -6.943 1.00 44 ATOM 1128 O GLU A 143 -1.699 85.596 -8.219 1.00 37 ATOM 1128 O GLU A 143 -1.699 85.596 -8.219 1.00 37 ATOM 1128 O GLU A 143 -1.699 85.596 -8.219 1.00 37 ATOM 1129 N GLN A 144 -1.699 85.596 -8.219 1.00 37 ATOM 1120 CA GLN A 144 -7.754 84.696 -9.888 1.00 37 ATOM 1131 CG GLN A 144 -7.754 84.696 -9.888 1.00 37 ATOM 1132 CG GLN A 144 -7.754 84.696 -9.888 1.00 37 ATOM 1133 N TYR A 145 -7.292 85.573 -9.099 1.00 7 ATOM 1134 OEI GLN A 144 -7.754 84.269 -9.309 1.00 37 ATOM 1135 N TYR A 145 -2.298 81.590 -7.239 1.00 2.00 37 ATOM 1136 C GLN A 144 -7.754 84.269 -9.878 1.00 37 ATOM 1137 N GL A 144 -7.754 84.269 -9.878 1.00 37 ATOM 1138 N TYR A 145 -0.226 77.7449 -7.024 1.00 37 ATOM 1136 C GLN A 144 -7.754 84.269 -9.898 1.00 37 ATOM 1137 N GL A 144 -8.522 83.352 -10.139 1.00 37 ATOM 1138 N TYR A 145 -0.227 77.549 77.939 1.00 37 ATOM 1139 N GL A 144 -8.522 83.350 -9.839 1.00 37 ATOM 1131 N TYR A 145 -0.895 79.930 -8.375 1.00 37 ATOM 1135 N TYR A 145 -0.228 77.7449 77.024 1.00 37 ATOM 1140 CB TYR A 145 -0.895 79.930 -8.375 1.00 37 ATOM 1141 ON TYR A 146 -0.895 8									1.00	37.91
ATOM 1113 C PHE A 141 -0.971 85.033 -10.969 1.00 31 ATOM 1114 O PHE A 141 -1.720 84.264 -10.369 1.00 32 ATOM 1115 N ALA A 142 0.162 85.993 -10.454 1.00 27 ATOM 1116 CA ALA A 142 0.657 85.091 -9.149 ATOM 1116 CA ALA A 142 1.969 85.792 -8.880 1.00 26 ATOM 1118 C ALA A 142 -0.917 85.313 -7.995 ATOM 1118 C ALA A 142 -0.37 85.313 -7.995 ATOM 1119 O ALA A 142 -0.38 84.480 -7.094 1.00 23 ATOM 1120 N GLU A 143 -1.013 86.437 -8.022 1.00 22 ATOM 1121 CA GLU A 143 -1.013 86.437 -8.022 1.00 22 ATOM 1122 CB GLU A 143 -1.03 86.750 -6.970 1.00 26 ATOM 1123 CG GLU A 143 -1.262 89.196 -6.990 1.00 31 ATOM 1124 CD GLU A 143 -1.733 90.618 -6.681 1.00 31 ATOM 1125 OEI GLU A 143 -2.921 90.916 -6.993 1.00 31 ATOM 1126 OE2 GLU A 143 -2.921 90.916 -6.943 1.00 34 ATOM 1127 C GLU A 143 -3.640 85.318 -5.999 1.00 31 ATOM 1128 OEI GLU A 143 -3.640 85.318 -5.999 1.00 31 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 33 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 33 ATOM 1128 OEI GLU A 143 -3.699 85.596 -8.219 1.00 33 ATOM 1128 OEI GLU A 143 -3.699 85.596 -8.299 1.00 33 ATOM 1128 OEI GLU A 143 -3.699 85.596 -8.299 1.00 33 ATOM 1130 CA GLN A 144 -3.699 85.596 -8.299 1.00 33 ATOM 1131 CB GLN A 144 -4.83 84.725 -8.392 1.00 2 ATOM 1131 CB GLN A 144 -4.83 84.725 -8.392 1.00 2 ATOM 1131 CB GLN A 144 -4.83 84.725 -8.392 1.00 35 ATOM 1133 CD GLN A 144 -4.893 84.725 -8.392 1.00 37 ATOM 1134 CB GLN A 144 -4.498 83.799 85.596 -9.309 1.00 37 ATOM 1135 CB GLN A 144 -4.498 83.799 85.596 -8.219 1.00 37 ATOM 1136 CB GLN A 144 -4.7922 85.573 -9.099 1.00 37 ATOM 1137 CB GLN A 144 -7.754 84.269 -9.309 1.00 37 ATOM 1138 N TYR A 145 -2.278 88 1.590 -7.239 1.00 37 ATOM 1136 CB GLN A 144 -7.754 84.269 -9.309 1.00 37 ATOM 1137 CB GLN A 144 -7.754 84.269 -9.309 1.00 37 ATOM 1138 N TYR A 145 -0.227 78.88 1.590 -7.944 1.00 37 ATOM 1136 CB GLN A 144 -7.754 84.266 -7.239 1.00 37 ATOM 1137 CB GLN A 144 -7.754 84.266 -7.239 1.00 37 ATOM 1138 N TYR A 145 -0.895 79.930 -8.047 1.00 37 ATOM 1136 CB TYR A 145 -0.895 79.930 -8.047 1.00 37 ATOM 1140 CB TYR A 145 -0.895 79.93								-12.349		36.70
ATOM 1114 O PHE A 141 -1.720 84.264 -10.369 1.00 34 ATOM 1115 N ALA A 142 0.162 83.493 -10.454 1.00 23 ATOM 1116 CA ALA A 142 0.657 85.931 -9.149 1.00 23 ATOM 1117 CB ALA A 142 1.969 85.792 -8.880 1.00 23 ATOM 1119 O ALA A 142 -0.317 85.313 -7.995 1.00 23 ATOM 1119 O ALA A 142 -0.317 85.313 -7.995 1.00 23 ATOM 1120 N GLU A 143 -1.033 86.437 -8.022 1.00 24 ATOM 1121 CA GLU A 143 -1.969 86.750 -6.970 1.00 23 ATOM 1122 CB GLU A 143 -2.403 88.211 -7.077 1.00 24 ATOM 1123 CG GLU A 143 -1.262 89.196 -6.890 1.00 34 ATOM 1124 CD GLU A 143 -1.262 89.196 -6.890 1.00 34 ATOM 1125 OEI GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1126 OEZ GLU A 143 -2.921 90.916 -6.943 1.00 34 ATOM 1127 C GLU A 143 -3.183 85.824 -7.018 1.00 34 ATOM 1128 O GLU A 143 -3.183 85.824 -7.018 1.00 34 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 34 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 34 ATOM 1130 CA GLN A 144 -3.699 85.596 -8.219 1.00 34 ATOM 1131 CB GLN A 144 -7.754 84.269 -9.858 1.00 37 ATOM 1132 CG GLN A 144 -8.83 84.725 -8.392 1.00 22 ATOM 1133 CB GLN A 144 -7.754 84.269 -9.809 1.00 37 ATOM 1134 OEI GLN A 144 -7.754 84.269 -9.9109 1.00 54 ATOM 1135 CB GLN A 144 -7.754 84.269 -9.9109 1.00 37 ATOM 1136 CB GLN A 144 -7.754 84.269 -9.9109 1.00 54 ATOM 1137 N GLN A 144 -7.754 84.269 -9.9109 1.00 54 ATOM 1138 N TYR A 145 -2.278 81.597 -9.099 1.00 37 ATOM 1138 N TYR A 145 -2.278 81.590 -7.239 1.00 2 ATOM 1138 N TYR A 145 -2.278 81.590 -7.239 1.00 2 ATOM 1137 N GLN A 144 -7.754 84.269 -9.109 1.00 54 ATOM 1138 N TYR A 145 -0.895 79.930 8.047 -9.835 1.00 2 ATOM 1136 C GLN A 144 -8.527 88.557 -7.944 1.00 2 ATOM 1137 N GLN A 144 -7.754 84.269 -9.109 1.00 54 ATOM 1138 N TYR A 145 -0.201 77.849 -7.934 1.00 2 ATOM 1136 C GLN A 144 -7.754 84.266 -7.239 1.00 3 ATOM 1137 N GLN A 144 -7.754 84.266 -9.858 1.00 3 ATOM 1138 N TYR A 145 -0.201 77.849 -7.934 1.00 2 ATOM 1139 N GLN A 144 -8.527 88.557 88.557 3.9099 1.00 3 ATOM 1140 CB TYR A 145 -0.895 79.930 -8.047 1.00 3.00 3.00 3.00 3.00 3.00 3.00 3.00							85.033	-10.969		31.10
ATOM 11.5 N ALA A 142 0.162 85.493 -10.454 1.00 23 ATOM 11.6 CA ALA A 142 0.657 85.091 -9.149 1.00 23 ATOM 11.7 CB ALA A 142 1.969 85.792 -8.880 1.00 26 ATOM 11.8 C ALA A 142 1.969 85.792 -8.880 1.00 26 ATOM 11.9 O ALA A 142 -0.317 85.313 -7.995 1.00 23 ATOM 11.20 N GLU A 143 -1.013 86.437 -8.022 1.00 24 ATOM 11.21 CA GLU A 143 -1.969 86.750 -6.970 1.00 24 ATOM 11.22 CB GLU A 143 -1.969 86.750 -6.970 1.00 24 ATOM 11.22 CB GLU A 143 -1.762 89.156 -6.890 1.00 24 ATOM 11.23 CG GLU A 143 -1.762 89.156 -6.890 1.00 34 ATOM 11.24 CD GLU A 143 -1.762 89.156 -6.890 1.00 34 ATOM 11.25 CBI GLU A 143 -0.906 91.448 -6.250 1.00 34 ATOM 11.26 CB2 GLU A 143 -0.906 91.448 -6.250 1.00 34 ATOM 11.27 C GLU A 143 -2.921 90.916 -6.943 1.00 34 ATOM 11.28 O GLU A 143 -3.690 85.318 -5.989 1.00 34 ATOM 11.29 N GLN A 144 -3.699 85.596 -8.219 1.00 34 ATOM 11.29 N GLN A 144 -3.699 85.596 -8.219 1.00 34 ATOM 11.30 CA GLN A 144 -5.275 84.696 -9.858 1.00 34 ATOM 11.31 CB GLN A 144 -6.520 83.852 -10.119 1.00 34 ATOM 11.32 CG GLN A 144 -6.529 83.852 -10.119 1.00 34 ATOM 11.33 CD GLN A 144 -6.520 83.852 -10.119 1.00 56 ATOM 11.33 CD GLN A 144 -6.520 83.852 -10.119 1.00 56 ATOM 11.34 CB GLN A 144 -6.520 83.852 -10.119 1.00 56 ATOM 11.35 NE2 GLN A 144 -6.520 83.852 -10.119 1.00 56 ATOM 11.36 CD GLN A 144 -6.520 83.852 -10.119 1.00 56 ATOM 11.37 NE2 GLN A 144 -6.520 83.852 -10.119 1.00 56 ATOM 11.38 NE2 GLN A 144 -6.520 83.852 -10.119 1.00 56 ATOM 11.39 CA GLN A 144 -7.754 84.269 -9.959 1.00 34 ATOM 11.31 CB GLN A 144 -7.754 84.269 -9.959 1.00 36 ATOM 11.33 CD GLN A 144 -7.754 84.269 -9.959 1.00 37 ATOM 11.34 NE2 GLN A 144 -7.754 84.269 -9.959 1.00 37 ATOM 11.35 NE2 GLN A 144 -7.754 84.269 -9.959 1.00 37 ATOM 11.36 CD GLN A 144 -7.754 84.269 -7.239 1.00 37 ATOM 11.37 NE2 GLN A 144 -7.754 84.269 -7.239 1.00 37 ATOM 11.39 CD GLN A 144 -7.754 84.269 -7.239 1.00 37 ATOM 11.39 CD GLN A 144 -7.754 84.269 -7.239 1.00 38 ATOM 11.30 NE2 GLN A 144 -7.754 84.269 -7.239 1.00 38 ATOM 11.30 NE2 GLN A 144 -7.754 84.269 -7.239 1.00 38 ATOM 11.30 NE2 GLN A 144 -7.7					141	-1.720				34.39
ATOM 1116 CA ALA A 142 0.667 85.091 91.199 1.00 24 ATOM 1117 CB ALA A 142 1.969 85.792 -8.880 1.00 26 ATOM 1118 C ALA A 142 -0.317 85.313 -7.995 1.00 23 ATOM 1119 O ALA A 142 -0.438 84.480 -7.094 1.00 23 ATOM 1121 CA GLU A 143 -1.013 86.437 -8.022 1.00 24 ATOM 1122 CB GLU A 143 -1.969 86.750 -6.970 1.00 24 ATOM 1122 CB GLU A 143 -2.403 88.211 -7.077 1.00 27 ATOM 1122 CB GLU A 143 -1.262 89.196 -6.891 1.00 34 ATOM 1122 CD GLU A 143 -1.262 89.196 -6.891 1.00 34 ATOM 1124 CD GLU A 143 -1.262 89.196 -6.891 1.00 34 ATOM 1125 OE1 GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1126 OE2 GLU A 143 -3.193 90.618 -6.681 1.00 34 ATOM 1126 OE2 GLU A 143 -3.183 85.824 -7.018 1.00 24 ATOM 1127 C GLU A 143 -3.160 85.318 -5.989 1.00 34 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 34 ATOM 1129 N GLU A 144 -3.699 85.596 8.219 1.00 34 ATOM 1130 CA GLU A 144 -3.699 85.596 8.219 1.00 34 ATOM 1131 CB GLU A 144 -7.527 84.696 -9.858 1.00 34 ATOM 1131 CB GLU A 144 -7.527 84.696 -9.858 1.00 34 ATOM 1131 CB GLU A 144 -7.527 84.696 -9.858 1.00 34 ATOM 1133 CD GLU A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1133 OCD GLU A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1131 OCD GLU A 144 -8.542 83.420 -8.876 1.00 3 ATOM 1135 OCD GLU A 144 -8.542 83.420 -8.876 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1137 O GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1137 O GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1136 C GLU A 144 -4.499 83.339 -7.938 1.00 3 ATOM 1140 C G TYR A 145 -0.207 7.949 1.00 3 ATOM 1141 C G TYR A 145 -0.307 7.941 1.00 3 ATOM 1141 C G TYR A 145 -0.307 7.941 1.00 3 ATOM 1141 C G TYR A 145 -0.307 7.941 1.00 3 ATOM 1141 C G TYR A 145 -0.30					142	0.162				27.56 23.24
ATOM 1117 CB ALA A 142 1.969 85.792 7.995 1.00 22 ATOM 1119 O ALA A 142 -0.438 84.480 -7.094 1.00 23 ATOM 1120 N GLU A 143 -1.033 86.437 -8.022 1.00 24 ATOM 1121 CA GLU A 143 -1.033 86.437 -8.022 1.00 24 ATOM 1122 CB GLU A 143 -1.038 86.437 -7.995 1.00 24 ATOM 1122 CB GLU A 143 -1.038 86.437 -7.995 1.00 24 ATOM 1122 CB GLU A 143 -1.262 89.196 -6.890 1.00 24 ATOM 1124 CD GLU A 143 -1.762 89.196 -6.890 1.00 34 ATOM 1125 CEI GLU A 143 -0.906 91.488 -6.255 1.00 44 ATOM 1126 OE2 GLU A 143 -0.906 91.488 -6.255 1.00 44 ATOM 1127 C GLU A 143 -2.921 90.916 -6.943 1.00 44 ATOM 1128 O GLU A 143 -3.183 85.824 -7.018 1.00 22 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 34 ATOM 1130 CA GLN A 144 -4.843 84.725 -8.392 1.00 34 ATOM 1131 CB GLN A 144 -5.275 84.696 -9.858 1.00 34 ATOM 1133 CD GLN A 144 -6.529 83.852 -10.139 1.00 34 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 5 ATOM 1135 NE2 GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 NA CEI GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1131 NA CEI GLN A 144 -7.754 84.269 -7.239 1.00 3 ATOM 1131 NA CEI GLN A 144 -7.754 84.269 -7.239 1.00 3 ATOM 1136 C GLN A 144 -7.754 84.269 -7.249 1.00 3 ATOM 1137 NA OEL GLN A 144 -7.754 84.269 -7.249 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1136 C GLN A 144 -7.754 84.269 -7.249 1.00 3 ATOM 1137 NA OEL GLN A 144 -7.754 84.269 -7.249 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 3 ATOM 1136 C GLN A 144 -7.754 84.269 -7.249 1.00 3 ATOM 1140 CB TYR A 145 -3.259 82.905 -8.351 1.00 3 ATOM 1140 CB TYR A 145 -3.259 82.905 -8.839 1.00 3 ATOM 1141 CD TYR A 145 -3.259 82.905 -8.839 1.00 3 ATOM 1140 CB TYR A 145 -3.259 82.905 -8.839 1.00 3 ATOM 1141 CD TYR A 145 -3.259 82.905 -8.839 1.00 3 ATOM 1149 O TYR A 146 -3.808 84.103 -7.934 1.00 3 ATOM 1149 O TYR A 146 -3.808 84.103 -7.944 1.00 3 ATOM 1150 CD TYR A 146 -3.808 8			CA	ALA A	142					26.02
ATOM 1118 C ALA A 142 -0.417 88.4.480 -7.094 1.00 22 ATOM 1119 O ALA A 142 -0.438 84.480 -7.094 1.00 22 ATOM 1120 N GLU A 143 -1.013 86.437 -8.022 1.00 24 ATOM 1121 CA GLU A 143 -1.969 86.750 -6.970 1.00 28 ATOM 1122 CB GLU A 143 -1.969 88.211 -7.077 1.00 27 ATOM 1123 CG GLU A 143 -1.262 89.196 -6.890 1.00 36 ATOM 1124 CD GLU A 143 -1.262 89.196 -6.890 1.00 36 ATOM 1125 OE1 GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1126 OE2 GLU A 143 -2.921 90.916 -6.943 1.00 36 ATOM 1127 C GLU A 143 -3.640 85.318 -5.989 1.00 32 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 32 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 32 ATOM 1130 CA GLN A 144 -6.529 85.596 -8.219 1.00 32 ATOM 1131 CB GLN A 144 -6.529 83.852 -10.139 1.00 32 ATOM 1132 CG GLN A 144 -7.754 84.269 -9.858 1.00 32 ATOM 1133 CB GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1134 OE1 GLN A 144 -7.922 83.852 -10.139 1.00 6 ATOM 1135 NEZ GLN A 144 -7.922 83.852 -10.139 1.00 6 ATOM 1136 C GLN A 144 -7.922 83.852 -10.139 1.00 6 ATOM 1137 NEZ GLN A 144 -7.925 83.852 -10.139 1.00 6 ATOM 1138 N TYR A 145 -3.259 82.573 90.999 1.00 7 ATOM 1138 N TYR A 145 -3.259 82.573 90.999 1.00 7 ATOM 1139 CA TYR A 145 -3.259 82.569 -7.239 1.00 32 ATOM 1140 CB TYR A 145 -1.393 81.286 8.505 1.00 32 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.835 1.00 32 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CG TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1140 CB TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CD TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1141 CD TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1145 CD TYR A 145 -0.895 79.930 -7.944 1.00 20 ATOM 1150 N TYR A 146 -2.390 82.546 -5.740 1.00 20 ATOM 1151 CD TYR A 146 -2.390 82.546 -5.740 1.00 20 ATOM 1151 CD TYR A 146 -		1117	CB							23.50
ATOM 1119 O ALA A 142 -1.013 86.437 -8.022 1.00 24 ATOM 1120 N GLU A 143 -1.013 86.437 -8.022 1.00 24 ATOM 1121 CA GLU A 143 -1.969 86.750 6.970 1.00 26 ATOM 1122 CB GLU A 143 -2.403 88.211 -7.077 1.00 27 ATOM 1123 CG GLU A 143 -2.403 88.211 -7.077 1.00 27 ATOM 1124 CD GLU A 143 -1.733 90.618 -6.681 1.00 36 ATOM 1125 OEI GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1126 OE2 GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1126 OE2 GLU A 143 -3.183 85.824 -7.018 1.00 22 ATOM 1128 O GLU A 143 -3.183 85.824 -7.018 1.00 22 ATOM 1128 O GLU A 143 -3.640 85.318 -5.999 1.00 31 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 31 ATOM 1130 CA GLN A 144 -6.527 84.696 -9.858 1.00 31 ATOM 1131 CB GLN A 144 -6.529 83.852 -10.139 1.00 32 ATOM 1131 CB GLN A 144 -6.529 83.852 -10.139 1.00 32 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.858 1.00 34 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.858 1.00 34 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7.7 ATOM 1136 CD GLN A 144 -7.922 85.573 -9.099 1.00 7.7 ATOM 1136 CD GLN A 144 -7.922 85.573 -9.099 1.00 7.7 ATOM 1137 O GLN A 144 -4.449 83.339 -7.938 1.00 2 ATOM 1136 CD GLN A 144 -7.922 85.573 -9.099 1.00 7.7 ATOM 1136 CD GLN A 144 -7.922 85.573 -9.099 1.00 7.7 ATOM 1136 CD GLN A 144 -7.922 85.573 -9.099 1.00 7.7 ATOM 1137 O GLN A 144 -7.792 85.573 -9.099 1.00 7.7 ATOM 1138 N TYR A 145 -3.259 82.905 8.335 1.00 2 ATOM 1137 O GLN A 144 -7.792 85.573 -7.998 1.00 3 ATOM 1140 CB TYR A 145 -3.259 82.905 8.335 1.00 2 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1144 CD2 TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1144 CD2 TYR A 145 -0.805 79.930 -8.047 1.00 1.00 ATOM 1144 CD2 TYR A 145 -0.805 79.830 -8.505 1.00 1.00 ATOM 1145 CE2 TYR A 145 -0.805 79.831 -0.505 1.00 1.00 ATOM 1145 CE2 TYR A 145 -0.805 79.831 -0.505 1.00 1.00 ATOM 1145 CE2 TYR A 145 -0.805 79.831 -0.505 1.00 1.00 ATOM 1145 CE2 TYR A 145 -0.805 79.831 -0.774 -0.24 1.00 1.00 ATOM 1145 CE2 TYR A 145 -0.805 79.831 -0.774 -0.24 1.00 1.00 ATOM 1145 CD2 TYR A 146 -0.805 83.991 -2.289 1.00 ATOM 1155 CD TYR A 146 -0.875 83.991 -2.289	ATOM	1118								23.30
ATOM 1120 N GLU A 143 -1.969 86.750 -6.970 1.00 22 ATOM 1121 CA GLU A 143 -1.969 86.750 -6.970 1.00 22 ATOM 1122 CB GLU A 143 -1.262 89.196 -6.890 1.00 36 ATOM 1124 CD GLU A 143 -1.733 90.618 -6.681 1.00 36 ATOM 1125 OE1 GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1126 OE2 GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1127 C GLU A 143 -2.921 90.916 -6.943 1.00 44 ATOM 1127 C GLU A 143 -3.640 85.318 -5.969 1.00 33 ATOM 1128 O GLU A 143 -3.640 85.318 -5.969 1.00 33 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 33 ATOM 1130 CA GLN A 144 -4.843 84.725 -8.392 1.00 2 ATOM 1131 CB GLN A 144 -5.275 84.696 -9.858 1.00 3 ATOM 1131 CB GLN A 144 -7.754 84.269 -9.309 1.00 5 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1135 NE2 GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 NE2 GLN A 144 -5.201 82.669 7.239 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1138 N TYR A 145 -0.0895 79.930 80.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1140 CB TYR A 145 -0.0895 79.930 8.335 1.00 2 ATOM 1140 CB TYR A 145 -0.200 70.895 79.930 8.047 1.00 2 ATOM 1141 CG TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1140 CB TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1141 CG TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1141 CC TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1141 CC TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1141 CC TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1141 CC TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1148 C TYR A 145 -0.200 70.895 79.930 -8.047 1.00 2 ATOM 1150 CR TYR A 146 -0.300 82.546 -5.740 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.	MOTA									24.11
ATOM 1122 CB GLU A 143 -2.403 88.211 -7.077 1.00 24 ATOM 1123 CG GLU A 143 -1.262 89.196 -6.890 1.00 31 ATOM 1124 CD GLU A 143 -1.733 90.618 -6.661 1.00 31 ATOM 1125 OE1 GLU A 143 -0.906 91.448 -6.250 1.00 41 ATOM 1126 OE2 GLU A 143 -2.921 90.916 -6.943 1.00 41 ATOM 1127 C GLU A 143 -3.183 85.824 -7.018 1.00 41 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 ATOM 1130 CA GLN A 144 -5.275 84.696 -9.858 1.00 ATOM 1131 CB GLN A 144 -6.529 83.852 -10.139 1.00 ATOM 1131 CB GLN A 144 -7.54 84.269 -9.309 1.00 ATOM 1133 CG GLN A 144 -7.754 84.269 -9.309 1.00 ATOM 1135 NE2 GLN A 144 -7.794 84.269 -9.309 1.00 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -5.275 83.690 -7.239 1.00 7 ATOM 1137 O GLN A 144 -5.276 83.352 -10.139 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 ATOM 1140 CB TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CG TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CG TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1140 CB TYR A 145 -1.393 81.590 -7.944 1.00 ATOM 1141 CD TYR A 145 -1.393 81.391 -7.938 1.00 ATOM 1146 CZ TYR A 145 -0.895 79.930 -8.047 1.00 ATOM 1146 CZ TYR A 146 -3.791 81.497 -7.219 1.00 ATOM 1150 CD TYR A 146 -3.791 81.497 -7.219 1.00 ATOM 1151 CB TYR A 146 -									1.00	26.83
ATOM 1123 CG GLU A 143 -1.262 89.196 -6.890 1.00 31 ATOM 1124 CD GLU A 143 -1.733 90.618 -6.681 1.00 32 ATOM 1125 OEI GLU A 143 -0.996 91.448 -6.250 1.00 44 ATOM 1126 OE2 GLU A 143 -0.996 91.448 -6.250 1.00 44 ATOM 1127 C GLU A 143 -3.183 85.824 -7.018 1.00 22 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 32 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 32 ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 32 ATOM 1130 CA GLN A 144 -4.843 84.725 -8.392 1.00 2 ATOM 1131 CB GLN A 144 -7.754 84.269 -9.858 1.00 3 ATOM 1131 CB GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1135 NE2 GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1136 C GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1137 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1137 C GLN A 144 -7.754 84.00 85.318 -7.938 1.00 2 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1137 C GLN A 144 -7.754 84.00 85.318 -7.994 1.00 3 ATOM 1136 C GLN A 144 -7.754 84.00 85.318 -7.994 1.00 3 ATOM 1137 C GLN A 144 -7.754 84.269 -7.299 1.00 3 ATOM 1136 C GLN A 144 -7.754 84.259 83.352 -10.139 1.00 5 ATOM 1137 C GLN A 144 -7.754 84.259 83.352 -10.139 1.00 6 ATOM 1136 C GLN A 144 -7.754 84.259 83.350 -7.994 1.00 2 ATOM 1137 C GLN A 144 -7.754 84.259 83.350 -7.994 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 3 ATOM 1140 CB TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1141 CG TYR A 145 -1.224 77.533 -7.846 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0								-7.077	1.00	27.46
ATOM 1125 OED GLU A 143 -1.733 90.618 -6.681 1.00 34 ATOM 1125 OED GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1126 OED GLU A 143 -0.906 91.448 -6.250 1.00 44 ATOM 1127 C GLU A 143 -2.921 90.916 -6.943 1.00 44 ATOM 1128 O GLU A 143 -3.183 85.824 -7.018 1.00 2.1 ATOM 1128 O GLU A 143 -3.699 85.596 -8.219 1.00 3. ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 3. ATOM 1130 CA GLN A 144 -5.275 84.696 -9.858 1.00 3. ATOM 1131 CB GLN A 144 -5.275 84.696 -9.858 1.00 3. ATOM 1131 CB GLN A 144 -7.754 84.269 -9.309 1.00 6. ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6. ATOM 1134 OEL GLN A 144 -8.542 83.420 -8.876 1.00 7. ATOM 1135 NEZ GLN A 144 -4.49 83.339 -7.938 1.00 2. ATOM 1136 C GLN A 144 -4.49 83.339 -7.938 1.00 2. ATOM 1137 O GLN A 144 -4.49 83.339 -7.938 1.00 2. ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2. ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 2. ATOM 1140 CB TYR A 145 -1.603 78.770 -8.356 1.00 2. ATOM 1141 CG TYR A 145 -1.603 78.770 -8.356 1.00 2. ATOM 1141 CD TYR A 145 -0.895 79.930 -8.047 1.00 2. ATOM 1144 CD TYR A 145 -0.221 79.814 -7.219 1.00 2. ATOM 1145 CEZ TYR A 145 -0.222 77.449 -7.024 1.00 2. ATOM 1146 CD TYR A 145 -0.221 79.814 -7.024 1.00 2. ATOM 1147 OH TYR A 145 -0.220 78.579 -6.705 1.00 2. ATOM 1149 O TYR A 145 -0.220 78.579 -6.705 1.00 2. ATOM 1140 CB TYR A 145 -0.221 79.814 -7.024 1.00 2. ATOM 1140 CB TYR A 145 -0.222 77.449 -7.024 1.00 2. ATOM 1140 CB TYR A 145 -0.220 76.231 -6.518 1.00 2. ATOM 1140 CD TYR A 145 -0.250 82.546 -5.740 1.00 2. ATOM 1140 CD TYR A 145 -0.250 82.546 -5.740 1.00 2. ATOM 1150 N TYR A 146 -1.933 83.931 -3.773 1.00 2. ATOM 1150 N TYR A 146 -1.652 83.991 -2.289 1.00 3. ATOM 1150 N TYR A 146 -1.652 83.991 -2.289 1.00 3. ATOM 1151 CA TYR A 146 -2.369 84.050 -1.807 1.00 1.00 3. ATOM 1151 CA TYR A 146 -3.697 84.050 -1.807 1.00 1.00 3.00 3.00 3.00 3.00 3.00 3.00								-6.890		30.94
ATOM 1125 OE1 GLU A 143 -0.906 91.448 -6.250 1.00 41 ATOM 1126 OE2 GLU A 143 -2.921 90.916 -6.943 1.00 41 ATOM 1127 C GLU A 143 -3.183 85.824 -7.018 1.00 22 ATOM 1128 O GLU A 143 -3.183 85.824 -7.018 1.00 23 ATOM 1129 N GLN A 144 -3.669 85.518 -5.989 1.00 33 ATOM 1129 N GLN A 144 -3.669 85.516 -8.219 1.00 33 ATOM 1130 CA GLN A 144 -1.843 84.725 -8.392 1.00 2 ATOM 1131 CB GLN A 144 -6.527 84.696 -9.858 1.00 3 ATOM 1131 CB GLN A 144 -6.529 83.852 -10.139 1.00 5 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1135 NE2 GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -4.449 83.319 -7.938 1.00 7 ATOM 1137 O GLN A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 3 ATOM 1137 C GLN A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1138 N TYR A 145 -1.393 81.286 -8.505 1.00 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 ATOM 1140 CB TYR A 145 -1.393 81.296 -8.355 1.00 2 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 ATOM 1141 CG TYR A 145 -1.393 81.286 -8.505 1.00 ATOM 1144 CD1 TYR A 145 -1.224 77.533 -7.846 1.00 1.00 ATOM 1145 CE2 TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1140 CD TYR A 145 -0.895 79.930 -6.705 1.00 ATOM 1145 CE2 TYR A 145 -0.221 79.814 -7.219 1.00 ATOM 1145 CE2 TYR A 145 -0.221 79.814 -7.219 1.00 ATOM 1145 CE2 TYR A 145 -0.221 79.814 -7.219 1.00 ATOM 1145 CE2 TYR A 145 -0.250 76.231 -6.518 1.00 ATOM 1145 CE2 TYR A 145 -0.250 76.231 -6.518 1.00 ATOM 1145 CE2 TYR A 145 -0.250 76.231 -6.518 1.00 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1150 N TYR A 146 -2.399 82.555 -4.283 1.00 ATOM 1150 N TYR A 146 -2.399 82.555 -4.283 1.00 ATOM 1150 N TYR A 146 -2.399 82.555 -4.283 1.00 ATOM 1150 N TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1150 N TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1150 N TYR A 146 -0.089 84.132 -0.458 1.00 ATOM 1150 N TYR A 146 -0.089 84.132 -0.458 1.00 ATOM 1150 N TYR A 146 -0.087 84.103 -0.002 -0.00 ATOM 1150 N TYR A 146 -0.087 84.103 -0.002						-1.733	90.618			36.67
ATOM 1126 OE2 GLU A 143 -2.921 90.916 -5.943 1.00 ATOM 1127 C GLU A 143 -3.183 85.824 -7.018 1.00 22 ATOM 1128 O GLU A 143 -3.640 85.318 -5.989 1.00 3. ATOM 1129 N GLN A 144 -3.699 85.596 -8.219 1.00 3. ATOM 1130 CA GLN A 144 -4.843 84.725 -8.392 1.00 2. ATOM 1131 CB GLN A 144 -6.5275 84.696 -9.858 1.00 3. ATOM 1131 CG GLN A 144 -6.529 83.852 -10.139 1.00 6. ATOM 1133 CG GLN A 144 -7.754 84.269 -9.309 1.00 6. ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6. ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6. ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7. ATOM 1136 C GLN A 144 -4.449 83.339 -7.938 1.00 2. ATOM 1136 C GLN A 144 -5.201 82.669 -7.239 1.00 3. ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2. ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 2. ATOM 1140 CB TYR A 145 -0.895 79.930 -8.047 1.00 2. ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2. ATOM 1141 CG TYR A 145 -1.393 81.286 -8.505 1.00 2. ATOM 1144 CD2 TYR A 145 -0.895 79.930 -8.047 1.00 2. ATOM 1144 CD2 TYR A 145 -0.221 79.814 -7.219 1.00 1.00 ATOM 1146 CZ TYR A 145 -0.221 79.814 -7.219 1.00 1.00 ATOM 1146 CZ TYR A 145 -0.250 76.231 -6.518 1.00 1.00 ATOM 1146 CZ TYR A 145 -0.250 76.231 -6.518 1.00 1.00 ATOM 1149 O TYR A 145 -2.798 81.487 -7.219 1.00 1.00 ATOM 1146 CZ TYR A 145 -0.250 76.231 -6.518 1.00 1.00 ATOM 1149 O TYR A 145 -0.250 76.231 -6.518 1.00 1.00 ATOM 1149 O TYR A 145 -0.250 76.231 -6.518 1.00 1.00 ATOM 1150 N TYR A 145 -0.250 76.231 -6.518 1.00 1.00 ATOM 1151 CA TYR A 146 -1.522 83.991 -3.773 1.00 ATOM 1151 CA TYR A 146 -1.652 83.991 -3.773 1.00 ATOM 1151 CA TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1151 CA TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1151 CA TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1151 CA TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1151 CA TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1151 CA TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1151 CA TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1151 CA TYR A 146 -0.087 84.256 -5.740 1.00 ATOM 1151 CA TYR A 146 -0.087 84.256 -5.740 1.00 ATOM 1151 CA TYR A 146 -0.087 84.256 -5.					143	-0.906				40.24
ATOM 1128				GLU A	143	-2.921				40.10 29.25
ATOM 1128 O GLU A 143 -3.640 85.318			С	GLU A	143					31.43
ATOM 1129 N GLN A 144 -1.843 84.725 -8.392 1.00 2 ATOM 1130 CA GLN A 144 -5.275 84.696 -9.858 1.00 3 ATOM 1131 CB GLN A 144 -5.275 84.696 -9.858 1.00 3 ATOM 1132 CG GLN A 144 -6.529 83.852 -10.139 1.00 6 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1134 OE1 GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1135 NE2 GLN A 144 -7.754 84.269 -9.309 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 O GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1138 N TYR A 145 -3.259 82.905 8.335 1.00 2 ATOM 1139 CA TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 CA TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -1.603 78.770 -8.356 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 1 ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1144 CD2 TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1146 CZ TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1146 CZ TYR A 145 -0.21 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 -0.221 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.0		1128	0							30.46
ATOM 1130 CA GLN A 144 -5.275 84.696 -9.858 1.00 3 ATOM 1131 CB GLN A 144 -6.529 83.852 -10.139 1.00 6 ATOM 1132 CG GLN A 144 -6.529 83.852 -10.139 1.00 6 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1134 OEI GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1135 NE2 GLN A 144 -8.542 83.420 -8.876 1.00 7 ATOM 1136 C GLN A 144 -4.449 83.339 -7.938 1.00 2 ATOM 1137 O GLN A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 2 ATOM 1140 CB TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 2 ATOM 1144 CD2 TYR A 145 -0.221 79.814 -7.219 1.00 3 ATOM 1144 CD2 TYR A 145 -0.221 79.814 -7.219 1.00 3 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1147 OH TYR A 145 -0.122 77.449 -7.024 1.00 3 ATOM 1148 C TYR A 145 -2.791 81.487 -7.024 1.00 3 ATOM 1148 C TYR A 145 -0.250 76.231 -6.518 1.00 3 ATOM 1149 O TYR A 145 -2.360 82.546 -5.740 1.00 3 ATOM 1149 O TYR A 145 -2.360 82.546 -5.740 1.00 3 ATOM 1150 N TYR A 146 -2.329 82.552 -4.283 1.00 3 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 3 ATOM 1150 C TYR A 146 -2.329 82.552 -4.283 1.00 3 ATOM 1151 CA TYR A 146 -2.691 84.023 -1.364 1.00 3 ATOM 1155 CD2 TYR A 146 -1.652 83.991 -2.289 1.00 3 ATOM 1159 OH TYR A 146 -0.088 84.103 -0.458 1.00 3 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.266 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1160 C TYR A 146 -3.859 82.822 -4.284 1.00 3 ATOM 1161 O TYR A 14	MOTA	1129								28.86
ATOM 1132 CB GLN A 144 -6.529 83.852 -10.139 1.00 5 ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1134 OE1 GLN A 144 -7.754 84.269 -9.309 1.00 7 ATOM 1135 NE2 GLN A 144 -7.754 84.269 -9.309 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 O GLN A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 2 ATOM 1140 CB TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 2 ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 12 ATOM 1144 CD2 TYR A 145 0.201 79.814 -7.219 1.00 ATOM 1145 CE2 TYR A 145 0.201 79.814 -7.219 1.00 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1147 OH TYR A 145 -2.791 81.487 -6.518 1.00 1.00 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 ATOM 1149 CD TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1152 CB TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1155 CE1 TYR A 146 -0.885 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1159 CF TYR A 146 -0.385 84.050 -1.807 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.807 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.807 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.807 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.807 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.050 -1.364 1.00 ATOM 1159 CF TYR A 146 -0.885 84.226 1.774 1.00 ATOM 1159 CF TYR A 146 -0.885 84.226 1.774 1.00 A	MOTA									38.80
ATOM 1133 CD GLN A 144 -7.754 84.269 -9.309 1.00 6 ATOM 1134 OE1 GLN A 144 -8.542 83.420 -8.876 1.00 7 ATOM 1135 NE2 GLN A 144 -8.542 83.420 -8.876 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1137 O GLN A 144 -4.449 83.339 -7.938 1.00 2 ATOM 1138 N TYR A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 2 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 2 ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1144 CD2 TYR A 145 -0.221 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1150 N TYR A 145 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1155 CB TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1155 CB TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CB TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CD TYR A 146 -2.369 84.023 -1.364 1.00 ATOM 1155 CD TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CD TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CD TYR A 146 -2.369 84.003 -1.807 1.00 ATOM 1155 CD TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CD TYR A 146 -2.491 84.003 -1.364 1.00 ATOM 1155 CD TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CD TYR A 146 -0.087 84.000 -1.807 1.00 ATOM 1155 CD TYR A 146 -0.875 84.206 1.774 1.00 ATOM 1155 CD TYR A 146 -0.875 84.206 1.774 1.00 ATOM 1155 CD TYR A 146 -0.875 84.206 1.774 1.00 ATOM 1156 CD TYR A 146 -0.875 84.206 -3.770 1.00 ATOM 1157 CD TYR A 146 -0.875 84.206 -3.770 1.00 ATOM 1150 N TYR A 146 -0.875 84.206 -3.770 1.00 ATOM 1150 N TYR A 146 -0.875 84.206 -3.770 1.00 ATOM 1150 N TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1150 N TYR								-10.139	1.00	58.07
ATOM 1134 OE1 GLN A 144 -8.542 83.420 -8.876 1.00 7 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 7 ATOM 1136 C GLN A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1137 O GLN A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 2 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1141 CG TYR A 145 -1.603 78.770 -8.356 1.00 2 ATOM 1142 CD1 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1144 CD2 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1145 CE2 TYR A 145 -0.221 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 1 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1147 OH TYR A 145 -2.791 81.487 -6.422 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1150 N TYR A 146 -2.360 82.552 -4.283 1.00 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1155 CB TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1155 CB TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1155 CB TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CC TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CC TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CC TYR A 146 -0.385 84.050 -1.807 1.00 ATOM 1155 CC TYR A 146 -0.385 84.050 -1.807 1.00 ATOM 1155 CC TYR A 146 -0.385 84.050 -1.807 1.00 ATOM 1155 CC TYR A 146 -0.385 84.050 -1.807 1.00 ATOM 1155 CC TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1155 CC TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1155 CC TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1156 CD TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1157 CC2 TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1160 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A							84.269	-9.309		67.99
ATOM 1135 NE2 GLN A 144 -7.922 85.573 -9.099 1.00 ATOM 1136 C GLN A 144 -4.449 83.339 -7.938 1.00 2 ATOM 1137 O GLN A 144 -5.201 82.669 -7.239 1.00 3 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 2 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 2 ATOM 1143 CE1 TYR A 145 -1.603 78.770 -8.356 1.00 1 ATOM 1144 CD2 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1145 CE2 TYR A 145 0.221 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 0.221 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1148 C TYR A 145 -2.791 81.487 -6.518 1.00 2 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 3 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 3 ATOM 1149 O TYR A 145 -2.360 82.546 -5.740 1.00 3 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 3 ATOM 1151 CA TYR A 146 -1.933 83.931 -3.773 1.00 3 ATOM 1152 CB TYR A 146 -1.933 83.931 -3.773 1.00 3 ATOM 1155 CG TYR A 146 -1.933 83.931 -3.773 1.00 3 ATOM 1155 CD TYR A 146 -0.088 84.132 -0.458 1.00 3 ATOM 1155 CD TYR A 146 -0.385 84.050 -1.807 1.00 3 ATOM 1155 CE2 TYR A 146 -0.088 84.132 -0.458 1.00 3 ATOM 1156 CD2 TYR A 146 -2.438 84.050 -1.807 1.00 3 ATOM 1158 CZ TYR A 146 -2.438 84.103 -0.002 1.00 3 ATOM 1159 OH TYR A 146 -2.438 84.103 -0.002 1.00 3 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 3 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 3 ATOM 1159 OH TYR A 146 -3.859 81.274 -2.967 1.00 3 ATOM 1150 N TRP A 147 -4.713 82.882 -4.284 1.00 3 ATOM 1160 C TYR A 146 -3.859 81.274 -2.967 1.00 3 ATOM 1160 N TRP A 147 -4.713 82.882 -4.284 1.00 3 ATOM 1160 N TRP A 147 -4.713 82.882 -4.284 1.00 3 ATOM 1160 CA TYR A 146 -3.859 81.274 -2.967 1.00 3 ATOM 1161 N TRP A 147 -6.087 82.620 -3.881 1.00 3 ATOM 1161 N TRP A 147 -6.087 82.620 -3.881 1.00 3 ATOM 1161 N TRP A 147 -6.087 82.620 -3.881 1.00 3 ATOM 1161 CA TYR A 147 -4.713 82.882 -4.284 1.00 3 ATOM 1161 CA TYR A 147 -6.087 82.620 -3.881 1.00 3 ATOM 1161 CA TYR A						-8.542	83.420			72.49
ATOM 1136 C GLN A 144 -4.449 83.339 -7.938 1.00 ATOM 1137 O GLN A 144 -5.201 82.669 -7.239 1.00 ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 ATOM 1139 CA TYR A 145 -2.788 81.590 -7.944 1.00 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 ATOM 1144 CD2 TYR A 145 -0.221 79.814 -7.219 1.00 ATOM 1145 CE2 TYR A 145 0.221 79.814 -7.219 1.00 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 ATOM 1147 OH TYR A 145 -2.791 81.487 -6.422 1.00 ATOM 1148 C TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1150 N TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1151 CA TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1153 CG TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1154 CD1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1158 CZ TYR A 146 -2.438 84.050 -1.807 1.00 ATOM 1159 OH TYR A 146 -2.879 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -2.879 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1159 OH TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1160 C TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1160 C TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1160 C TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.885 81.274 -2.967 1.00 ATOM 1161 O TYR A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00					144	-7.922				74.56 25.81 .
ATOM 1138 N TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1139 CA TYR A 145 -3.259 82.905 -8.335 1.00 2 ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 2 ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1144 CD2 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1145 CE2 TYR A 145 0.221 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 0.221 79.814 -7.219 1.00 2 ATOM 1146 CZ TYR A 145 0.21 77.449 -7.024 1.00 2 ATOM 1147 OH TYR A 145 0.250 76.231 -6.518 1.00 2 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 2 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 3 ATOM 1150 N TYR A 146 -2.320 82.546 -5.740 1.00 3 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 3 ATOM 1153 CG TYR A 146 -1.933 83.931 -3.773 1.00 3 ATOM 1155 CB TYR A 146 -1.933 83.991 -2.289 1.00 3 ATOM 1155 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 3 ATOM 1155 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 3 ATOM 1156 CD2 TYR A 146 -2.438 84.103 -0.002 1.00 3 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 3 ATOM 1158 CZ TYR A 146 -2.438 84.103 -0.002 1.00 3 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 3 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 3 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1160 C TYR A 146 -3.859 84.226 1.774 1.00 3 ATOM 1161 O TYR A 146 -3.859 84.226 -3.881 1.00 3 ATOM 1161 O TYR A 146 -3.859 84.226 -3.881 1.00 3 ATOM 1161 O TYR A 146 -3.859 84.226 -3.881 1.00 3 ATOM 1161 O TYR A 146 -3.859 84.226 -3.881 1.00 3 ATOM 1161 O TYR A 146 -3.859 84.226 -3.881 1.00 3 ATOM 1161 O TYR A 146 -3.859 84.226 -3.881 1.00 3 ATOM 1163 CA TRP A 147 -4.713 82.882 -4.284 1.00 3 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 3 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 3 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 3 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 3				GLN A	144					30.61
ATOM 1138 N TYR A 145 -3.259 82.39 82.39 82.70		1137	0	GLN A						26.62
ATOM 1140 CB TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -1.393 81.286 -8.505 1.00 2 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 1 ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1144 CD2 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1144 CD2 TYR A 145 0.221 79.814 -7.219 1.00 2 ATOM 1145 CE2 TYR A 145 0.607 78.579 -6.705 1.00 2 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1147 OH TYR A 145 0.250 76.231 -6.518 1.00 2 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 2 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 2 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 2 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 2 ATOM 1152 CB TYR A 146 -1.652 83.991 -2.289 1.00 2 ATOM 1155 CG1 TYR A 146 -0.088 84.132 -0.458 1.00 2 ATOM 1155 CD2 TYR A 146 -0.088 84.132 -0.458 1.00 2 ATOM 1155 CD2 TYR A 146 -2.438 84.050 -1.807 1.00 2 ATOM 1155 CD2 TYR A 146 -2.438 84.103 -0.002 1.00 2 ATOM 1155 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 2 ATOM 1155 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 2 ATOM 1155 CD2 TYR A 146 -2.438 84.103 -0.002 1.00 2 ATOM 1155 CD2 TYR A 146 -2.438 84.103 -0.002 1.00 2 ATOM 1159 OH TYR A 146 -2.875 84.226 1.774 1.00 2 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 2 ATOM 1160 C TYR A 146 -3.859 81.274 -2.967 1.00 2 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 2 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 2 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 2 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 2 ATOM 1163 CA TRP A 147 -4.713 82.882 -4.284 1.00 2 ATOM 1163 CA TRP A 147 -4.713 82.882 -4.284 1.00 2 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 2 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 2 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 2 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 2	ATOM `	1138	N							22.39
ATOM 1140 CB TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1141 CG TYR A 145 -0.895 79.930 -8.047 1.00 2 ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 ATOM 1144 CD2 TYR A 145 0.221 79.814 -7.219 1.00 2 ATOM 1145 CE2 TYR A 145 0.607 78.579 -6.705 1.00 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 ATOM 1147 OH TYR A 145 0.250 76.231 -6.518 1.00 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1152 CB TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1153 CG TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1159 OH TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1160 C TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.088 83.752 -4.363 1.00	MOTA									21.02
ATOM 1142 CD1 TYR A 145 -1.603 78.770 -8.356 1.00 24 1.00 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 12 144 CD2 TYR A 145 0.221 79.814 -7.219 1.00 24 1.00 14 145 CE2 TYR A 145 0.607 78.579 -6.705 1.00 1.00 14 145 CE2 TYR A 145 0.607 78.579 -6.705 1.00 1.00 14 146 CZ TYR A 145 0.507 76.231 -6.518 1.00 14 147 OH TYR A 145 0.250 76.231 -6.518 1.00 14 148 C TYR A 145 -2.791 81.487 -6.422 1.00 14 148 C TYR A 145 -3.231 80.482 -5.875 1.00 14 149 O TYR A 145 -3.231 80.482 -5.875 1.00 14 149 O TYR A 146 -2.360 82.546 -5.740 1.00 14 150 N TYR A 146 -2.360 82.546 -5.740 1.00 14 151 CA TYR A 146 -2.329 82.552 -4.283 1.00 151 CA TYR A 146 -1.933 83.931 -3.773 1.00 152 CB TYR A 146 -1.652 83.991 -2.289 1.00 153 CG TYR A 146 -0.345 84.050 -1.807 1.00 154 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 155 CE1 TYR A 146 -0.345 84.050 -1.807 1.00 155 CE1 TYR A 146 -2.691 84.023 -1.364 1.00 156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 158 CZ TYR A 146 -2.438 84.103 -0.002 1.00 158 CZ TYR A 146 -3.704 82.193 -3.770 1.00 158 CZ TYR A 146 -3.704 82.193 -3.770 1.00 158 CZ TYR A 146 -3.859 81.274 -2.967 1.00 150 ATOM 1159 OH TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1160 C TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 -4.360 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 -4.360 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 -4.360 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 -4.360 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 -4.361 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 -4.361 1.00 ATOM									1.00	23.34
ATOM 1143 CE1 TYR A 145 -1.224 77.533 -7.846 1.00 1 ATOM 1144 CD2 TYR A 145 0.221 79.814 -7.219 1.00 2 ATOM 1145 CE2 TYR A 145 0.607 78.579 -6.705 1.00 2 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 2 ATOM 1147 OH TYR A 145 0.250 76.231 -6.518 1.00 2 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 2 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 2 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 2 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 2 ATOM 1152 CB TYR A 146 -1.933 83.931 -3.773 1.00 2 ATOM 1153 CG TYR A 146 -1.652 83.991 -2.289 1.00 2 ATOM 1154 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 2 ATOM 1155 CE1 TYR A 146 -0.345 84.050 -1.807 1.00 2 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 2 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 2 ATOM 1158 CZ TYR A 146 -2.438 84.103 -0.002 1.00 2 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 2 ATOM 1159 OH TYR A 146 -3.859 84.226 1.774 1.00 2 ATOM 1160 C TYR A 146 -3.859 84.226 1.774 1.00 2 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 2 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 2 ATOM 1163 CA TRP A 147 -4.713 82.882 -4.284 1.00 2 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 2 ATOM 1163 CA TRP A 147 -6.087 83.752 -4.363 1.00								-8.356	1.00	21.49
ATOM 1144 CD2 TYR A 145 0.221 79.814 -7.219 1.00 24 ATOM 1145 CE2 TYR A 145 0.607 78.579 -6.705 1.00 24 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 25 ATOM 1147 OH TYR A 145 0.250 76.231 -6.518 1.00 25 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 25 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1152 CB TYR A 146 -1.933 83.931 -3.773 1.00 ATOM 1153 CG TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1155 CE1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1160 C TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00							77.533	-7.846		19.67
ATOM 1145 CE2 TYR A 145 0.607 78.579 -6.705 1.00 24 ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 27 ATOM 1147 OH TYR A 145 0.250 76.231 -6.518 1.00 27 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 27 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 27 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1152 CB TYR A 146 -1.933 83.931 -3.773 1.00 ATOM 1153 CG TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1154 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1159 OH TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00							79.814			23.57
ATOM 1146 CZ TYR A 145 -0.122 77.449 -7.024 1.00 ATOM 1147 OH TYR A 145 0.250 76.231 -6.518 1.00 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1152 CB TYR A 146 -1.933 83.931 -3.773 1.00 ATOM 1153 CG TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1154 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1159 OH TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1160 C TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1161 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1162 N TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00					145	0.607				20.74 20.82
ATOM 1147 OH TYR A 145 0.250 76.231 -6.348 1.00 ATOM 1148 C TYR A 145 -2.791 81.487 -6.422 1.00 ATOM 1149 O TYR A 145 -3.231 80.482 -5.875 1.00 ATOM 1150 N TYR A 146 -2.360 82.546 -5.740 1.00 ATOM 1151 CA TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1152 CB TYR A 146 -1.933 83.931 -3.773 1.00 ATOM 1153 CG TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1154 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00			CZ	TYR A	145					24.24
ATOM 1148 C TYR A 145 -2.791 81.487 -0.422			OH	TYR A						22.08
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ATOM 1150 N TYR A 146 -2.329 82.552 -4.283 1.00 ATOM 1151 CA TYR A 146 -1.933 83.931 -3.773 1.00 ATOM 1152 CB TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1153 CG TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1154 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00	MOTA									20.10
ATOM 1152 CB TYR A 146 -1.933 83.931 -3.773 1.00 ATOM 1153 CG TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1153 CG TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CE1 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -6.087 82.822 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.820 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00									1.00	16.74
ATOM 1152 CB TYR A 146 -1.652 83.991 -2.289 1.00 ATOM 1153 CG TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1154 CD1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CE1 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -6.087 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00								-3.773	1.00	15.16
ATOM 1154 CD1 TYR A 146 -0.345 84.050 -1.807 1.00 ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CE2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00					_			-2.289		19.44
ATOM 1155 CE1 TYR A 146 -0.088 84.132 -0.458 1.00 ATOM 1155 CE2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00							84.050			19.08
ATOM 1156 CD2 TYR A 146 -2.691 84.023 -1.364 1.00 ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00										17.67
ATOM 1157 CE2 TYR A 146 -2.438 84.103 -0.002 1.00 ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00										18.53 17.70
ATOM 1158 CZ TYR A 146 -1.137 84.161 0.437 1.00 ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00		•								19.52
ATOM 1159 OH TYR A 146 -0.875 84.226 1.774 1.00 ATOM 1160 C TYR A 146 -3.704 82.193 -3.770 1.00 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00				TYR A						25.01
ATOM 1160 C TYR A 146 -3.704 82.193 3.704 ATOM 1161 O TYR A 146 -3.859 81.274 -2.967 1.00 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00										17.31
ATOM 1161 O TYR A 146 -3.833 02.11 ATOM 1162 N TRP A 147 -4.713 82.882 -4.284 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -4.363 1.00		1160								21.09
ATOM 1162 N TRP A 147 -4.713 32.620 -3.881 1.00 ATOM 1163 CA TRP A 147 -6.087 82.620 -3.881 1.00	MOTA									17.15
ATOM 1163 CA TREE 147 6 988 83.752 -4.363 1.00									1.00	17.97
ATOM 1164 CD								-4.363	1.00	14.43
	ATOM	1164	CB							

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MOTA	1165	CG	TRP A	147	-6.580	85.045	-3.742	1.00	16.44
ATOM	1166	CD2	TRP A	147	-6.371	85.292	-2.353	1.00	15.61
ATOM	1167	CE2	TRP A	147	-5.855	86.588	-2.222	1.00	13.55
ATOM ATOM	1168	CE3	TRP A	147	-6.556	84.520	-1.195	1.00	13.91
ATOM	1169 1170	CD1 NE1	TRP A	147	-6.209	86.192	-4.389	1.00	17.35
ATOM	1171	CZ2	TRP A	147 147	-5.760	87.122	-3.482	1.00	16.82
ATOM	1172	CZ3	TRP A	147	-5.526 -6.225	87.138	-0.999	1.00	15.71
ATOM	1173	CH2	TRP A	147	-5.714	85.066 86.365	0.023	1.00	13.54
ATOM	1174	C	TRP A	147	-6.589	81.238	0.114 -4.308	1.00	14.81
ATOM	1175	0	TRP A	147	-7.401	80.620	-3.611	1.00 1.00	19.27
ATOM	1176	N	ASP A	148	-6.059	80.731	-5.416	1.00	19.35 18.47
ATOM	1177	CA	ASP A	148	-6.416	79.405	-5.904	1.00	19.12
ATOM	1178	CB	ASP A	148	-5.801	79.141	-7.275	1.00	24.71
MOTA	1179	CG	ASP A	148	-6.709	79.536	-8.404	1.00	26.35
ATOM ATOM	1180	OD1	ASP A	148	-7.852	79.946	-8.136	1.00	32.40
ATOM	1181 1182	OD2 C	ASP A ASP A	148	-6.284	79.423	-9.569	1.00	32.06
ATOM	1183	0	ASP A	148 148	-5.973 -6.707	78.328	-4.927	1.00	18.33
ATOM	1184	N	VAL A	149	-6.797 -4.679	77.536 78.2 7 6	-4.486	1.00	23.56
ATOM	1185	CA	VAL A	149	-4.193	77.281	-4.603 -3.647	1.00	18.47
MOTA	1186	CB	VAL A	149	-2.678	77.225	-3.513	1.00	15.91 14.54
ATOM	1187	CG1	VAL A	149	-2.136	76.214	-4.447	1.00	17.43
MOTA	1188	CG2	VAL A	149	-2.055	78.590	-3.729	1.00	16.13
ATOM	1189	С	VAL A	149	-4.757	77.549	-2.271	1.00	18.11
ATOM	1190	0	VAL A	149	-4.897	76.633	-1.467	1.00	21.98
ATOM ATOM	1191 1192	N CA	PHE A	150	-5.032	78.814	-1.979	1.00	20.18
ATOM	1193	CB	PHE A	150 150	-5.629 -5.931	79.173	-0.703	1.00	21.84
ATOM	1194	CG	PHE A	150	-6.441	80.666 81.152	-0.669 0.651	1.00	19.11
ATOM	1195	CD1	PHE A	150	-5.572	81.689	1.586	1.00	22.86 22.65
MOTA	1196	CD2	PHE A	150	-7.794	81.091	0.955	1.00	26.06
ATOM	1197	CE1	PHE A	150	-6.045	82.158	2.800	1.00	26.82
ATOM	1198	CE2	PHE A	150	-8.274	81.561	2.171	1.00	22.46
ATOM ATOM	1199 1200	CZ C	PHE A	150	-7.400	82.093	3.091	1.00	25.45
ATOM	1201	0	P8E A PHE A	150 150	-6.933 -7.214	78.382	-0.581	1.00	24.16
MOTA	1202	N	GLY A	151	-7.715	77.769 78.379	0.453 -1.656	1.00	28.22
ATOM	1203	CA	GLY A	151	-8.970	77.659	-1.656	1.00	22.56 20.54
ATOM	1204	C	GLY A	151	-8.761	76.182	-1.417	1.00	21.70
ATOM	1205	0	GLY A	151	-9.504	75.565	-0.654	1.00	25.57
ATOM ATOM	1206	N	LEU A	152	-7.745	75.610	-2.049	1.00	18.26
ATOM	1207 1208	CA CB	LEU A LEU A	152 152	-7.460	74.193	-1.876	1.00	19.08
ATOM	1209	CG	LEU A	152	-6.304 -5.838	73.770 72.318	-2.782	1.00	19.81
ATOM	1210	CD1	LEU A	152	-6.969	71.381	-2.680 -3.103	1.00	19.38
MOTA	1211	CD2	LEU A	152	-4.615	72.127	-3.538	1.00	16.96 11.13
ATOM	1212	C	LEU A	152	-7.093	73.916	-0.425	1.00	24.24
ATOM	1213	0	LEU A	152	-7.667	73.032	0.219	1.00	26.47
ATOM ATOM	1214	N	SER A	153	-6.141	74.682	0.095	1.00	24.56
ATOM	1215 1216	CA CB	SER A SER A	153	-5.687	74.517	1.468	1.00	22.73
ATOM	1217	OG	SER A	153 153	-4.591 -3.572	75.528	1.770	1.00	21.22
ATOM	1218	c	SER A	153	-6.842	75.448 74.665	0.787 2.444	1.00	21.77
ATOM	1219	0	SER A	153	-7.041	73.823	3.316	1.00	22.43 24.75
ATOM	1220	N	SER A	154	-7.642	75.698	2.245	1.00	22.50
ATOM	1221	CA	SER A	154	-8.792	75.950	3.088	1.00	25.72
ATOM	1222	CB	SER A	154	-9.588	77.108	2.497	1.00	25.08
ATOM ATOM	1223 1224	og C	SER A SER A		-10.672	77.472	3.328	1.00	38.08
ATOM	1225	0	SER A	154 154	-9.662 -10.140	74.688 74.356	3.218	1.00	29.51
ATOM	1226	N	ALA A	155	-9.786	73.941	4.310 2.121	1.00 1.00	33.28
MOTA	1227	CA	ALA A		-10.582	72.713	2.099	1.00	31.53 29.45
ATOM	1228	CB	ALA A	155	-11.038	72.396	0.696	1.00	30.93
ATOM	1229	C	ALA A	155	-9.846	71.523	2.683	1.00	28.62
ATOM ATOM	1230	0	ALA A		-10.473	70.657	3.281	1.00	32.89
ATOM	1231 1232	N CA	LEU A LEU A	156 156	-8.530 -7.730	71.455	2.485	1.00	28.48
ATOM	1232	CB	LEU A	156	-7.739 -6.323	70.355 70.368	3.032	1.00	23.61
ATOM	1234	CG	LEU A	156	-6.043	69.867	2.476 1.061	1.00	23.88
ATOM	1235	CD1.	LEU A	156	-4.587	70.132	0.729	1.00 1.00	20.69 20.27
ATOM	1236	CD2	LEU A	156	-6.325	68.394	0.958	1.00	20.27
ATOM	1237	C	LEU A	156	-7.688	70.488	4.547	1.00	25.37

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ATOM	1238	0	LEU A	156	-7.558	69.490	5.262	1.00	26.18
ATOM	1239	N	LEU A	157	-7.773	71.726	5.036	1.00	25.81
ATOM	1240	CA	LEU A	157	-7.770	71.981	6.474	1.00	25.36
ATOM	1241	CB	LEU A	157	-7.557	73.466	6.775	1.00	19.73 16.53
ATOM	1242	CG	LEU A	157	-6.135 -6.111	74.027 75.418	6.673 7.270	1.00 1.00	17.68
ATOM ATOM	1243 1244	CD1 CD2	LEU A LEU A	157 157	-5.165	73.418	7.431	1.00	15.33
ATOM	1245	C	LEU A	157	-9.076	71.470	7.107	1.00	29.31
ATOM	1246	ō	LEU A	157	-9.111	71.079	8.279	1.00	32.51
MOTA	1247	N	LYS A	158	-10.161	71.500	6.341	1.00	33.23
ATOM	1248	CA	LYS A	158	-11.442	70.982	6.814	1.00	31.84
MOTA	1249	CB	LYS A	158	-12.553	71.355	5.837 5.745	1.00 1.00	33.31 34.09
ATOM	1250	CG	LYS A LYS A	158 158	-12.780 -13.850	72.845 73.167	4.738	1.00	41.31
ATOM ATOM	1251 1252	CD CE	LYS A	158	-14.186	74.649	4.754	1.00	47.04
ATOM	1253	NZ	LYS A	158	-15.362	74.923	3.886	1.00	56.43
ATOM	1254	С	LYS A	158	-11.289	69.460	6.905	1.00	30.71
MOTA	1255	0	LYS A	158	-11.770	68.836	7.848	1.00	34.49
ATOM	1256	N	GLY A	159	-10.570	68.884	5.942	1.00	30.71
ATOM	1257	CA	GLY A	159	-10.313	67.453 67.040	5.930 7.111	1.00	28.93 30.81
ATOM ATOM	1258 1259	C 0	GLY A GLY A	159 159	-9.447 -9.690	66.003	7.732	1.00	34.67
ATOM	1260	N	TYR A	160	-8.440	67.851	7.431	1.00	28.73
ATOM	1261	CA	TYR A	160	-7.556	67.575	8.556	1.00	29.15
ATOM	1262	CB	TYR A	160	-6.378	68.554	8.556	1.00	29.86
ATOM	1263	CG	TYR A	160	-5.181	68.055	7.780	1.00	28.35
ATOM	1264	CD1	TYR A	160	-4.828	68.607 68.124	6.543 5.830	1.00 1.00	26.01 25.65
ATOM	1265 1266	CE1 CD2	TYR A TYR A	160 160	-3.727 -4.412	67.017	8.279	1.00	26.25
ATOM ATOM	1265	CE2	TYR A	160	-3.321	66.530	7.584	1.00	26.20
ATOM	1268	CZ	TYR A	160	-2.977	67.076	6.365	1.00	28.06
ATOM	1269	ОН	TYR A	160	-1.884	66.546	5.711	1.00	25.91
ATOM	1270	C	TYR A	160	-8.313	67.646	9.884	1.00	32.18
ATOM	1271	0	TYR A	160	-8.034	66.884 68.571	10.812 9.976	1.00 1.00	33.45 33.22
ATOM	1272	N CA	ALA A ALA A	161 161	-9.262 -10.074	68.734	11.180	1.00	30.35
ATOM ATOM	1273 1274	CB	ALA A	161	-10.995	69.919	11.021	1.00	30.11
ATOM	1275	C	ALA A	161	-10.890	67.470	11.433	1.00	31.40
MOTA	1276	0	ALA A	161	-10.863	66.911	12.525	1.00	32.99
ATOM	1277	N	LEU A	162	-11.593	67.012	10.405	1.00	30.20
ATOM	1278	CA	LEU A	162	-12.405	65.813 65.587	10.50 1 9.186	1.00	31.99 32.01
MOTA MOTA	1279 1280	CB CG	LEU A LEU A	162 162	-13.156 -14.116	66.719	8.801	1.00	33.82
ATOM	1281	CD1	LEU A	162	-14.867	66.349	7.545	1.00	34.17
MOTA	1282	CD2	LEU A	162	-15.096	66.997	9.933	1.00	34.51
ATOM	1283	C	LEU A	162	-11.580	64.580	10.877	1.00	32.42
MOTA	1284	0	LEU A	162	-12.002	63.767	11 .696	1.00	35.19 34.99
ATOM	1285	N	ALA A	163	-10.396 -9.504	64.453 63.325	10.291 10.573	1.00	32.51
ATOM ATOM	1286 1287	CA CB	ALA A ALA A	163		63.395	9.670	1.00	28.78
ATOM	1288	C	ALA A	163		63.273	12.038	1.00	30.64
ATOM	1289	0	ALA A	163	-8.745	62.217	12.571	1.00	30.60
ATOM	1290	N	LEU A	164		64.428	12.674	1.00	29.60
ATOM	1291	CA	LEU A	164		64.478 65.666	14.054 14.274	1.00 1.00	30.80 30.81
ATOM	1292	CB CG	LEU A LEU A	164 164		65.550	13.570	1.00	29.00
ATOM ATOM	1293 1294	CD1	LEU A	164		66.875	13.576	1.00	30.09
ATOM	1295	CD2	LEU A	164		64.509	14.245	1.00	28.45
ATOM	1296	С	LEU A	164	-9.778	64.529	14.993	1.00	34.67
MOTA	1297	0	LEU A	164		64.811	16.179	1.00	37.15
ATOM	1298	N	GLY A	165		64.258 64.258	14.455 15.265	1.00 1.00	35.40 34.11
ATOM	1299	CA C	GLY A GLY A		-12.172 -12.637	65.606	15.781	1.00	35.01
MOTA MOTA	1300 1301	0	GLY A		-13.465	65.680	16.694	1.00	38.99
ATOM	1302	N	LYS A		-12.111	66.678	15.208	1.00	34.42
ATOM	1303	CA	LYS A		-12.490	68.021	15.619	1.00	34.45
MOTA	1304	СВ	LYS A		-11.267	68.924	15.571	1.00	31.93
MOTA	1305	CG	LYS A		-10.232	68.560	16.594 17.956	1.00 1.00	32.57 34.75
MOTA	1306	CD	LYS A LYS A	166	-10.711 -9.756	68.973 68.522	19.022	1.00	34.75
ATOM ATOM	1307 1308	CE NZ	LYS A		-9.736	69.161	20.313	1.00	40.84
ATOM	1309	C	LYS A		-13.557	68.535	14.666	1.00	37.47
ATOM	1310	o	LYS A		-13.825	67.901	13.642	1.00	41.52

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ATOM	1311	N	GLU A	167	-14.189	69.660	14.994	1.00	38.98
MOTA	1312	CA	GLU A	167	-15.202	70.205	14.094	1.00	41.09
ATOM	1313	CB	GLU A	167	-15.947	71.398	14.713	1.00	45.19
ATOM	1314	CG	GLU A	167	-15.110	72.638	15.025	1.00	55.15
ATOM	1315	CD	GLU A	167	-14.565	72.661	16.448	1.00	61.94
ATOM	1316	OE1	GLU A	167	-14.113	73.742	16.887	1.00	62.92
ATOM	1317	OE2	GLU A	167	-14.584	71.611	17.131	1.00	64.60
ATOM ATOM	1318 1319	C 0	GLU A GLU A	167	-14.525	70.605	12.780	1.00	41.39
ATOM	1320	И	GLU A	167 168	-13.339 -15.285	70.935 70.581	12.761 11.692	1.00 1.00	41.98
ATOM	1321	CA	GLU A	168	-t4.779	70.918	10.365	1.00	39.45 38.77
ATOM	1322	CB	GLU A	168	-15.943	70.959	9.387	1.00	40.01
ATOM	1323	CG	GLU A	168	-15.535	70.844	7.951	1.00	42.60
ATOM	1324	CD	GLU A	168	-16.721	70.635	7.056	1.00	45.09
ATOM	1325	OE1	GLU A	168	-17.408	71.626	6.740	1.00	51.44
ATOM	1326	OE2	GLU A	168	-16.979	69.477	6.677	1.00	50.69
ATOM	1327	C	GLU A	168	-13.965	72.212	10.255	1.00	37.65
ATOM ATOM	1328 1329	N O	GLU A ASN A	168 169	~12.966 ~14.389	72.270 73.247	9.533	1.00	37.39
MOTA	1330	CA	ASN A	169	-13.696	74.527	10.965 10.925	1.00 1.00	34.88
ATOM	1331	CB	ASN A	169	-14.710	75.654	10.976	1.00	31.36 38.29
ATOM	1332	CG	ASN A	169	-15.529	75.726	9.732	1.00	46.39
ATOM	1333	OD1	ASN A	169	-14.993	75.919	8.646	1.00	52.41
MOTA	1334	ND2	ASN A	169	-16.833	75.544	9.865	1.00	52.70
ATOM	1335	C	ASN A	169	-12.677	74.717	12.029	1.00	29.02
ATOM	1336	0	ASN A	169	-12.264	75.839	12.318	1.00	25.13
ATOM	1337	N	PHE A	170	-12.236	73.618	12.617	1.00	29.52
ATOM ATOM	1338 1339	CA CB	PHE A PHE A	170 170	-11.276 -10.938	73.687	13.702	1.00	30.89
ATOM	1340	CG	PHE A	170	-10.938	72.275 72.248	14.191 15.377	1.00	34.08
ATOM	1341	CD1	PHE A	170	-10.418	72.827	16.575	1.00	38.01 41.53
ATOM	1342	CD2	PHE A	170	-8.778	71.658	15.293	1.00	39.11
ATOM	1343	CE1	PHE A	170	-9.571	72.824	17.675	1.00	40.36
ATOM	1344	CE2	PHE A	170	-7.925	71.649	16.385	1.00	41.21
ATOM	1345	CZ	PHE A	170	-8.326	72.235	17.580	1.00	42.47
ATOM	1346	С	PHE A	170	-10.012	74.464	13.305	1.00	32.24
ATOM	1347	0	PHE A	170	-9.496	75.255	14.102	1.00	32.82
ATOM ATOM	1348	N	PHE A PHE A	171	-9.537	74.269	12.072	1.00	30.18
ATOM	1349 1350	CA CB	PHE A	171 171	-8.338 -7.436	74.959 74.018	11.595 10.780	1.00	25.80
ATOM	1351	CG	PHE A	171	-6.801	72.922	11.584	1.00	21.23 17.74
ATOM	1352	CD1	PHE A	171	-6.984	71.592	11.232	1.00	19.14
ATOM	1353	CD2	PHE A	171	-6.028	73.212	12.699	1.00	20.58
MOTA	1354	CE1	PHE A	171	-6.409	70.559	11.986	1.00	19.44
ATOM	1355	CE2	PHE A	171	-5.449	72.188	13.457	1.00	19.74
ATOM	1356	CZ	PHE A	171	-5.644	70.861	13.095	1.00	18.77
ATOM	1357	C	PHE A	171	-8.720	76.142	10.722	1.00	27.98
ATOM ATOM	1358 1359	O N	PHE A ALA A	171	-8.301 -9.573	77.282	10.968	1.00	26.96
ATOM	1360	Q	ALA A	172 172	-9.573 -10.009	75.874 76. 8 80	9.737 8.770	1.00 1.00	27.10
ATOM	1361	CB	ALA A	172	-10.996	76.276	7.798	1.00	23.60 20.83
ATOM	1362	C	ALA A	172	-10.542	78.191	9.310	1.00	25.20
ATOM	1363	0	ALA A	172	-10.477	79.204	8.623	1.00	27.68
MOTA	1364	N	ARG A	173	-11.044	78.195	10.540	1.00	27.56
MOTA	1365	CA	MG A	173	-11.573	79.429	11.098	1.00	28.04
ATOM	1366	CB	ARG A	173	-12.374	79.170	12.377	1.00	29.47
ATOM	1367	CG	ARG A	173	-11.559	79.001	13.633	1.00	35.23
ATOM ATOM	1368	CD	MG A	173	-12.452	78.858	14.868	1.00	40.18
ATOM .	1369 1370	NE CZ	MG A ARG A	173 173	-12.898 -14.162	77.482 77.074	15.106 15.017	1.00	44.83
ATOM	1371	NH1	MG A	173	-15.122	77.934	14.695	1.00	48.14 48.64
ATOM	1372	NH2	MG A	173	-14.468	75.800	15.240	1.00	44.20
ATOM	1373	C	MG A	173	-10.433	80.401	11.355	1.00	30.23
ATOM	1374	0	ARG A	173	-10.657	81.591	11.584	1.00	32.24
ATOM	1375	N	HIS A	174	-9.206	79.889	11.314	1.00	28.30
ATOM	1376	CA	HIS A	174	-8.023	80.713	11.537	1.00	28.03
ATOM	1377	CB	HIS A	174	-7.051	79.999	12.473	1.00	25.87
ATOM	1378	CG	HIS A	174	-7.622	79.688	13.816	1.00	26.33
ATOM	1379	CD2	HIS A	174	-8.121	78.536	14.326	1.00	28.81
ATOM ATOM	1380 1381	ND1 CE1	HIS A HIS A	174 174	-7.705 -8.228	80.623 80.059	14.826	1.00	27.96
ATOM	1381	NE2	HIS A	174	-8.228 -8.488	80.059 78. 7 93	15.900 15.624	1.00	28.08 27.09
ATOM	1382	C	HIS A	174	-7.305	81.064	10.235	1.00	27.63
		_						1.00	~

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ATOM	138-	4 0	HIS A	174	-6.371	0: 0==			
ATOM	138	5 ท	PHE A				10.240	1.00	31.26
ATOM	1386						9.138	1.00	26.90
ATOM					-7.165	90.631	7.801	1.00	
	1381	_	PHE A	175	-7.222	79.289	7.074		22.15
ATOM	1388	_		175	-6.293	79.176		1.00	21.26
ATOM	1389	CD:	PHE A	175	-6.652		5.911	1.00	23.40
ATOM	1390					78.420	4.803	1.00	20.93
ATOM	1391			175	-5.046	79.781	5.931	1.00	
ATOM				175	-5.789	78.266	3.741		19.53
	1392			175	-4.170	79.630		1.00	19.79
ATOM	1393	CZ	PHE A	175	-4.545		4.866	1.00	19.63
MOTA	1394	C	PHE A	175		78.870	3.770	1.00	19.09
ATOM	1395		PBE A		-8.030	81.655	7.071	1.00	23.58
ATOM	1396			175	-9.032	81.299	6.443	1.00	
			LYS A	176	-7.636	82.923	7.136		25.37
ATOM	1397	CA	LYS A	176	-8.412	84.004		1.00	22.96
ATOM	1398	CB	LYS A	176	-8.991		6.529	1.00	26.79
ATOM	1399		LYS A			84.922	7.619	1.00	32.23
ATOM	1400			176	-9.711	84.185	8.752	1.00	
		CD	LYS A	176	-10.312	85.139	9.782		37.22
ATOM	1401	CE	LYS A	176	-9.271 -	86.065		1.00	45.14
ATOM	1402	NZ	LYS A	176	-8.282		10.408	1.00	51.76
ATOM	1403	C	LYS A			85.352	11.277	1.00	54.44
ATOM	1404	ō		176	-7.624	84.842	5.529	1.00	
ATOM			LYS A	176	-6.447	85.150	5.736		26.95
	1405	N	PRO A	177	-8.308	85.327		1.00	29.87
ATOM	1406	CD	PRO A	177	-9.714		4.485	1.00	24.40
ATOM	1407	CA	PRO A			85.067	4.146	1.00	20.13
ATOM	1408	CB		177	-7.685	86.133	3.445	1.00	
ATOM			PRO A	177	-8.838	86.376	2.481		19.31
	1409	CG	PRO A	177	-9.687	85.187		1.00	16.22
ATOM	1410	C	PRO A	177	-7.084		2.664	1.00	13.22
ATOM	1411	0	PRO A	177		87.434	3.903	1.00	21.14
ATOM	1412	N	ASP A		-6.096	87.883	3.349	1.00	25.46
ATOM	1413			178	-7.660	88.049	4.917	1.00	
		CA	ASP A	178	-7.145	89.341	5.355		26.69
ATOM	1414	CB	ASP A	178	-8.220	90.162		1.00	30.90
ATOM	1415	CG	ASP A	178	-8.927		6.073	1.00	40.73
ATOM	1416	ODl	ASP A			89.377	7.153	1.00	58.65
ATOM	1417			178	-9.660	88.411	6.813	1.00	
ATOM		OD2	ASP A	178	-8.754	89.731	8.344		67.55
	1418	C	ASP A	178	-5.891	89.303		1.00	69.29
ATOM	1419	0	ASP A	178	-5.154		6.183	1.00	25.93
ATOM	1420	N	ASP A	179		90.282	6.225	1.00	27.92
ATOM	1421	CA			-5.620	88.180	6.828	1.00	20.77
ATOM					-4.432	88.129	7.645	1.00	
	1422	CB	ASP A	179	-4.790	88.332	9.120		20.37
ATOM	1423	CG	ASP A		-5.553	87.157		1.00	24.28
ATOM	1424	ODl			-5.957		9.717	1.00	28.49
ATOM	1425	OD2				86.249	8.967	1.00	32.76
ATOM	1426	C			-5.750	87.134	10.953	1.00	
ATOM				179	-3.550	86.912	7.499		34.31
	1427	0	ASP A	179	-2.568	86.807		1.00	20.24
ATOM	1428	N	THR A		-3.870	05.007	8.224	1.00	22.73
ATOM	1429	CA				85.996	6.587	1.00	18.73
ATOM	1430	CB			-3.035	84.809	6.453	1.00	19.30
ATOM				180 -	-3.533	83.818	5.372	1.00	
	1431	OG1		L80 -	-2.592	82.741	5.254		20.49
ATOM	1432	CG2	THR A		-3.657			1.00	20.62
ATOM	1433	C				84.488	4.024	1.00	18.20
ATOM	1434	0			1.577	85.144	6.173	1.00	22.74
ATOM	1435				1.269	86.060	5.407	1.00	
ATOM		N		.81 -	0.689	84.402	6.826		23.45
	1436	CA	LEU A 1		0.752	84.558		1.00	22.30
MOTA	1437	CB			1.450		6.661	1.00	19.63
ATOM	1438	CG				84.460	8.023	1.00	11.22
ATOM	1439				1.280	85.655	8.947	1.00	8.88
ATOM		CD1		81	1.760	85.318	10.332		
	1440	CD2	LEU A 1	81	2.041	86.823		1.00	7.59
ATOM	1441	C	LEU A 1	_	1.315		8.395	1.00	9.34
ATOM	1442	0				83.488	5.702	1.00	19.45
ATOM	1443		.		2.524	83.287	5.629	1.00	22.17
ATOM				82	0.441	82.775	5.003		
	1444			82	0.886	81.749	4.072	1.00	15.84
ATOM	1445	CB	ALA A 1		0.306	81.111		1.00	13.71
ATOM	1446							1.00	15.01
ATOM	1447				1.797	82.379	3.017	1.00	16.85
ATOM	1448				1.690	83.571	2.723	1.00	
ATOM					2.679	81.583	2.429		15.28
	1449		SER A 18	33 3	3.584	82.108		1.00	15.86
ATOM	1450	CB :	SER A 18				1.416	1.00	14.12
ATOM	1451		SER A 18			82.430	2.039	1.00	12.59
ATOM	1452					81.250	2.497	1.00	13.59
ATOM			SER A 18			81.130	0.257	1.00	
	1453		SER A 18	3 3		79.923	0.422		13.98
ATOM	1454	и , и	/AL A 18	4 4		81.674		1.00	17.17
ATOM	1455	CA (AL A 18				-0.931	1.00	15.35
ATOM	1456					80.885	-2.133	1.00	13.86
	-	(/AL A 18	* 3	.366	81.361	-3.335	1.00	
									13.35

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						500	-4.554	1.00	11.12
2004	1457	CG1 V	AL A	184	3.625	80.500	-2.994	1.00	14.34
ATOM ATOM	1458		AL A	184	1.907	81.283	-2.479	1.00	13.94
ATOM	1459		/AL A	184	5.698	81.161 82.314	-2.459	1.00	15.07
ATOM	1460		AL A	184	6.123	80.107	-2.722	1.00	16.12
ATOM	1461		JAL A	185	6.469 7.871	80.237	-3.095	1.00	18.01
ATOM	1462		VAL A	185	8.818	79.516	-2.096	1.00	19.45
MOTA	1463		VAL A	185	10.262	79.683	-2.528	1.00	14.07
MOTA	1464	•	VAL A	185 185	8.629	80.054	-0.708	1.00	17.49 18.98
ATOM	1465		VAL A VAL A	185	8.039	79.551	-4.438	1.00	20.19
ATOM	1466	-	VAL A	185	7.660	78.391	-4.585	1.00 1.00	22.23
MOTA	1467	-	LEU A	186	8.541	80.282	-5.428	1.00	22.67
ATOM	1468 1469	•	LEU A	186	8.781	79.717	-6.760 7.861	1.00	17.46
ATOM	1469		LEU A	186	8.468	80.748	-7.861 -7.844	1.00	17.76
MOTA	1471	CG	LEU A	186	7.117	81.480	-9.092	1.00	19.25
ATOM	1472	CD1	LEU A	186	6.993	82.315	-7.761	1.00	12.57
MOTA MOTA	1473	CD2	LEU A	186	5.970	80.514 79.325	-6.800	1.00	21.43
ATOM	1474	С	LEU A	186	10.261	80.169	-7.058	1.00	21.60
ATOM	1475	0	LEU A	186	11.124	78.065	-6.500	1.00	18.26
ATOM	1476	N	ILE A	187	10.555 11.929	77.586	-6.477	1.00	18.51
ATOM	1477	CA	ILE A	187	12.068	76.373	-5.547	1.00	17.33
ATOM	1478	C8	ILE A	187	13.524	75.915	-5.484	1.00	17.55
MOTA	1479	CG2	ILE A	187	11.560	76.727	-4.152	1.00	14.78
ATOM	1480	CG1	ILE A	187 187	11.608	75.582	-3.201	1.00	12.56
MOTA	1481	CDI	ILE A		12.421	77.183	-7.858	1.00	24.55 28.10
MOTA	1482	C	ILE A	_	11.688	76.567	-8.632	1.00	27.00
MOTA	1483	0	ARG A		13.671	77.509	-8.158	1.00	27.28
MOTA	1484	N	ARG A		14.258	77.160	-9.447	1.00	25.39
MOTA	1485	CA CB	ARG A		14.659	78.405	-10.241	1.00	26.11
ATOM	1486	CG	ARG A	_	15.481	78.037	-11.466	1.00	26.92
MOTA	1487	CD	ARG A		16.122	79.207	-12.169	1.00	33.43
MOTA	1488 1489	NE	ARG P				-13.448 -14.176	1.00	37.61
ATOM	1490	CZ	ARG F				-13.779	1.00	40.25
ATOM	1491	NHl	MG				-15.327	1.00	45.39
ATOM	1492	NH2	ARG A	A 188		- 4 001	-9.302	1.00	27.56
MOTA MOTA	1493	С	ARG I			- 4 650	-8.644	1.00	28.16
ATOM	1494	0	ARG			75.120	-9.921	1.00	28.98
ATOM	1495	N	TYR		15.463		-9.901	1.00	30.35
MOTA	1496	Q	TYR				-9.600	1.00	28.57
ATOM	1497	C8	TYR				-8.179	1.00	27.58
ATOM	1498	CG	TYR				-7.862	1.00	30.42
ATOM	1499	CD1	TYR				-6.555	1.00	32.46 25.30
MOTA	1500	CE1	TYR TYR				-7.154	1.00	27.43
ATOM	1501	CD2	TYR			000	-5.846	1.00	31.28
ATOM	1502	CE2	TYR			6 72.182	-5.553	1.00 1.00	37.45
ATOM	1503	OH	TYR			4 71.980	-4.262	1.00	30.75
MOTA	1504	C	TYR			25 74.335	-11.293	1.00	31.49
MOTA	1505		TYR			73.905		1.00	29.84
MOTA	1506 1507		PRO		0 18.39			1.00	29.04
MOTA	1508		PRO		90 19.1			1.00	29.41
ATOM	1509		PRO	A 1	90 19.1	001		1.00	30.04
MOTA	1510		PRO	A 1	90 20.1			1.00	27.63
MOTA MOTA	1511		PRC		90 20.5			1.00	29.09
ATOM	1512	_	PRC	-	90 19.8			1.00	31.04
MOTA	1513	_	PRO		90 20.1			1.00	27.02
ATOM	1514	4 N		• • • •	91 20.2 91 21.0			1.00	25.82
MOTA	1519	5 CA						1.00	24.40
ATOM	151	6 CB					6 -17.164	1.00	23.94
MOTA	151				191 21.6 191 21.9			1.00	24.85
MOTA	151				191 22.5		9 -17.370	1.00	26.57
MOTA	151			• • •	191 22.		-18.169	1.00	24.25 22.72
MOTA	152				191 23.		-18.764	1.00	
ATOM	152				191 23.	769 70.37		1.00	
MOTA	152			-	191 24.	791 69.65			
MOTA	152	-		TR A	191 22.	406 73.73			
MOTA	152			r A	191 22.	477 74.8			
MOTA	152 152			EU A	192 23.	453 73.1	31 -14.620	1.00	
ATOM	153		A L	EU A			14 -14.662	1.00	
ATOM	15	_		EU A			78 -13.322 86 -12.789	1.00	
MOTA MOTA	15			EU A	192 24	.221 75.4	UU -12.705		
Alon									

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ATOM	1530	CD1	LEU A	192	24.644	75.909	-11.386	1.00	20.65
ATOM	1531	CD2	LEU A	192	24.252	76.664	-13.738	1.00	21.14
ATOM	1532	С	LEU A	192	25.856	72.673	-15.013	1.00	34.74
ATOM	1533	0	LEU A	192	25.803	71.511	-14.586	1.00	33.09
MOTA	1534	И	ASP A	193	26.778	73.085	-15.867	1.00	36.86
ATOM	1535	CA	ASP A	193	27.877	72.250	-16.289	1.00	42.70 48.25
ATOM	1536	CB	ASP A	193	27.564	71.544 70.728	-17.600 -18.106	1.00 1.00	52.17
ATOM	1537 1538	CG OD1	ASP A ASP A	193 193	28.732 29.125	70.728	-19.271	1.00	58.38
ATOM ATOM	1536	OD1	ASP A	193	29.266	69.897	-17.338	1.00	53.48
ATOM	1540	C	ASP A	193	29.032	73.196	-16.494	1.00	42.38
ATOM	1541	0	ASP A	193	29.061	73.951	-17.461	1.00	46.89
ATOM	1542	N	PRO A	194	29.994	73.178	-15.574	1.00	40.26
ATOM	1543	CD	PRO A	194	31.206	74.016	-15.565	1.00	40.20
ATOM	1544	CA	PRO A	194	29.956	72.294	-14.414	1.00	38.87
ATOM	1545	CB	PRO A	194	31.419	72.224	-14.018 -14.250	1.00 1.00	39.32 39.54
ATOM	1546	CG	PRO A	194	31.863 29.082	73.644 72.863	-13.293	1.00	40.57
ATOM	1547 1548	с 0	PRO A PRO A	194 194	28.773	74.065	-13.261	1.00	39.81
ATOM ATOM	1549	И	TYR A	195	28.667	71.005	-12.395	1.00	38.88
ATOM	1550	CA	TYR A	195	27.826	72.341	-11.269	1.00	35.95
ATOM	1551	CB	TYR A	195	26.869	71.187	-10.933	1.00	33.96
ATOM	1552	CG	TYR A	195	25.572	71.600	-10.255	1.00	33.27
ATOM	1553	CD1	TYR A	195	24.390	71.688	-10.984	1.00	32.32
MOTA	1554	CE1	TYR A	195	23.200	72.048	-10.381	1.00	31.47
ATOM	1555	CD2	TYR A	195	25.522	71.887	-8.889	1.00	29.66
ATOM	1556	CE2	TYR A	195	24.330	72.249 72.325	-8.276 -9.030	1.00	27.38 27.54
ATOM	1557	CZ OH	TYR A TYR A	195 195	23.178 21.996	72.665	-8.436	1.00	25.96
ATOM ATOM	1558 1559	C	TYR A	195	28.726	72.624	-10.072	1.00	35.66
ATOM	1560	0	TYR A	195	29.616	71.832	-9.748	1.00	34.39
ATOM	1561	N	PRO A	196	28.505	73.762	-9.402	1.00	34.12
MOTA	1562	CD	PRO A	196	27.458	74.742	-9.730	1.00	32.84
ATOM	1563	CA	PRO A	196	29.270	74.183	-8.231	1.00	34.92
MOTA	1564	CB	PRO A	196	28.472	75.377	-7.735	1.00	35.33
MOTA	1565	CG	PRO A	196	27.915	75.951	-8.995	1.00	36.48 40.87
ATOM	1566	C	PRO A	196 196	29.276 28.257	73.076 72.808	-7.188 -6.558	1.00	44.01
ATOM ATOM	1567 1568	о N	PRO A GLU A	197	30.418	72.425	-7.013	1.00	46.54
ATOM	1569	CA	GLU A	197	30.535	71.337	-6.048	1.00	49.40
ATOM	1570	CB	GLU A	197	31.992	70.896	-5.916	1.00	59.62
ATOM	1571	CG	GLU A	197	32.595	70.350	-7.211	1.00	74.74
ATOM	1572	CD	GLU A	197	34.093	70.061	-7.108	1.00	82.34
MOTA	1573	OE1	GLU A	197	34.807	70.797	-6.383	1.00	86.57
MOTA	1574	OE2	GLU A	197	34.558	69.100	-7.765	1.00 1.00	87.43 45.50
ATOM	1575	C	GLU A	197	30.007 29.395	71.757 70.972	-4.692 -3.985	1.00	46.60
ATOM	1576	и	GLU A ALA A	197 198	30.216	73.018	-4.352	1.00	43.56
ATOM ATOM	1577 1578	CA	ALA A	198	29.765	73.538	-3.072	1.00	42.05
ATOM	1579	CB	ALA A	198	30.214	74.968	-2.908	1.00	42.58
ATOM	1580	C	ALA A	198	28.264	73.443	-2.861	1.00	41.83
ATOM	1581	0	ALA A	198	27.805	73.315	-1.728	1.00	46.61
ATOM	1582	N	ALA A	199	27.501	73.501	-3.946	1.00	36.04
ATOM	1583	CA	ALA A	199	26.052	73.450	-3.852	1.00	32.51
ATOM	1584	CB	ALA A	199	25.430	74.173	-5.019 -3.772	1.00	33.11 33.23
ATOM	1585	C	ALA A ALA A	199 199	25.512 24.307	72.044 71.837	-3.900	1.00	38.62
ATOM	1586 1587	O N	ILE A	200	26.397	71.075	-3.590	1.00	32.94
ATOM ATOM	1588	CA	ILE A	200	25.973	69.687	-3.508	1.00	34.13
ATOM	1589	CB	ILE A		26.565	68.846	-4.644	1.00	30.62
ATOM	1590	CG2	ILE A	200	26.086	67.409	-4.527	1.00	19.56
ATOM	1591	CG1	ILE A	200	26.154	69.451	-5.988	1.00	31.15
MOTA	1592	CD1	ILE A	200	27.065	69.109	-7.124	1.00	34.14
ATOM	1593	C	ILE A	200	26.353	69.073	-2.182	1.00	37.98 42.30
ATOM	1594	0	ILE A	200	27.525	68.817	-1.909 -1.356	1.00 1.00	42.30
ATOM	1595	N	LYS A LYS A	201 201		68.844 68.258	-0.045	1.00	42.08
ATOM	1596	CA CB	LYS A			68.776	0.935	1.00	44.17
ATOM ATOM	1597 1598	CG	LYS A	201		70.275	1.203	1.00	47.76
ATOM	1599	CD	LYS A	201		70.918	1.218	1.00	52.10
ATOM	1600	CE	LYS A	201		72.423	1.021	1.00	52.22
ATOM	1601	NZ	LYS A	201		73.026	0.955	1.00	52.59
ATOM	1602	C	LYS A	201	25.443	66.761	-0.179	1.00	39.59

ATOM	1603	О	LYS A	201	24.587	66.255	-0.886	1.00	42.27
ATOM	1604	N	THR A	202	26.338	66.052	0.485	1.00	40.47
ATOM	1605	CA	THR A	202	26.329	64.605	0.424	1.00	42.05
ATOM	1606	CB	THR A	202	27.682	64.062	-0.114	1.00	38.96
ATOM	1607	OG1	THR A	202	27.900	62.727	0.356	1.00	42.95
ATOM	1608	CG2	THR A	202	28.838	64.970	0.276	1.00	40.84
ATOM	1609	C	THR A	202	25.908	64.022	1.781	1.00	42.98
ATOM ATOM	1610	N	THR A	202	26.553	64.247	2.809	1.00	47.33
MOTA	1611 1612	CA	ALA A ALA A	203 203	24.750 24.195	63.369	1.785	1.00	41.07
ATOM	1613	Q	ALA A	203	24.195	62.776 62.179	2.995 2.713	1.00	42.49
ATOM	1614	Ĉ	ALA A	203	25.110	61.705	3.525	1.00	36.69 44.40
MOTA	1615	0	ALA A	203	25.924	61.159	2.787	1.00	45.26
ATOM	1616	N	ALA A	204	24.920	61.348	4.788	1.00	47.23
ATOM	1617	CA	ALA A	204	25.733	60.316	5.408	1.00	47.81
ATOM	1618	Q	ALA A	204	25.266	60.089	6.817	1.00	48.23
MOTA	1619	С	ALA A	204	25.701	59.000	4.615	1.00	48.73
ATOM	1620	0	ALA A	204	26.680	58.252	4.581	1.00	51.77
ATOM	1621	N	ASP A	205	24.574	58.725	3.970	1.00	45.72
ATOM	1622	CA	ASP A	205	24.437	57.501	3.189	1.00	42.78
ATOM ATOM	1623 1 624	CB CG	ASP A	205	22.984	56.989	3.221	1.00	47.36
ATOM	1625	OD1	ASP A ASP A	205 205	22.018 22.374	57.827	2.370	1.00	50.09
ATOM	1626	OD2	ASP A	205	20.880	58.937 57.362	1.922 2.147	1.00	54.80
ATOM	1627	C	ASP A	205	24.915	57.644	1.751	1.00	48.85
ATOM	1628	0	ASP A	205	24.628	56.787	0.924	1.00 1.00	39.10
ATOM	1629	N	GLY A	206	25.597	58.744	1.447	1.00	39.36 37.66
ATOM	1630	CA	GLY A	206	26.100	58.968	0.097	1.00	36.43
ATOM	1631	С	GLY A	206	25.238	59.669	-0.950	1.00	34.15
ATOM	1632	0	GLY A	206	25.739	60.024	-2.017	1.00	31.94
ATOM	1633	N	THR A	207	23.956	59.877	-0.679	1.00	29.49
ATOM	1634	CA	THR A	207	23.109	60.538	-1.657	1.00	25.87
ATOM	1635	CB	THR A	207	21.637	60.442	-1.260	1.00	27.03
ATOM	1636	OG1	THR A	207	21.345	59.109	-0.824	1.00	29.78
ATOM	1637	CG2	THR A	207	20.766	60.752	-2.447	1.00	28.36
ATOM	1638	C	THR A	207	23.509	61.998	-1.837	1.00	25.47
ATOM	1639	0	THR A	207	23.891	62.663	-0.881	1.00	27.07
ATOM ATOM	1640 1641	N CA	LYS A LYS A	208 208	23.481	62.478	-3.073	1.00	26.75
ATOM	1642	Q	LYS A	208	23.828 24.323	63.866 64.035	-3.347 -4.785	1.00	28.57
ATOM	1643	ČG	LYS A	208	25.565	63.216	-5.112	1.00	34.36 40.54
ATOM	1644	CD	LYS A	208	26.734	63.592	-4.210	1.00	53.48
ATOM	1645	CE	LYS A	208	27.937	62.669	-4.416	1.00	58.70
MOTA	1646	NZ	LYS A	208	29.114 .	63.071	-3.586	1.00	62.46
ATOM	1647	C	LYS A	208	22.540	64.626	-3.124	1.00	27.85
ATOM	1648	0	LYS A	208	21.497	64.231	-3.638	1.00	29.27
ATOM	1649	Ŋ	LEU A	209	22.620	65.743	-2.413	1.00	25.63
ATOM	1650	CA	LEU A	209	21.442	66.518	-2.066	1.00	18.54
ATOM	1651	CB	LEU A	209	21.149	66.348	-0.583	1.00	15.76
ATOM ATOM	1652	CG	LEU A	209	21.027	64.949	-0.009	1.00	16.54
ATOM	1653 1654	CD1 CD2	LEU A LEU A	209 209	21.176 19.704	65.029	1.478	1.00	19.47
ATOM	1655	C	LEU A	209	21.570	64.330 67.997	-0.393 -2.303	1.00	14.83
ATOM	1656	0	LEU A	209	22.647	68.561	-2.184	1.00	19.56 20.20
ATOM	1657	N	SER A	210	20.438	68.624	-2.591	1.00	20.20
ATOM	1658	CA	SER A	210	20.359	70.064	-2.782	1.00	26.32
ATOM	1659	CA	SER A	210	19.243	70.433	-3.770	1.00	26.58
ATOM	1660	OG	SER A	210	19.611	70.186	-5.115	1.00	34.59
ATOM	1661	С	SER A	210	20.000	70.625	-1.407	1.00	26.44
MOTA	1662	0	SER A	210	20.466	71.694	-1.023	1.00	29.35
ATOM	1663	N	PHE A	211	19.143	69.900	-0.683	1.00	27.04
ATOM	1664	CA	PHE A	211	18.691	70.296	0.652	1.00	24.33
ATOM	1665	CB	PHE A	211	17.306	70.938	0.603	1.00	25.32
ATOM	1666	CG CD1	PHE A	211	17.275	72.243	-0.123	1.00	27.69
ATOM ATOM	1667	CD1 CD2	PHE A PHE A	211 211	16.682	72.341	-1.378	1.00	35.01
ATOM	1668 1669	CD2	PHE A	211	17.867 16.681	73.370 73.547	0.426	1.00	31.73
ATOM	1670	CE2	PHE A	211	17.875	74.586	-2.082 -0.269	1.00	35.58
ATOM	1671	CZ	PHE A	211	17.281	74.672	-1.525	1.00 1.00	34.04
ATOM	1672	C	PHE A	211	18.670	69.116	1.611	1.00	36.38 24.35
ATOM	1673	o	PHE A	211	18.062	68.076	1.339	1.00	21.15
ATOM	1674	N	GLU A	212	19.354	69.304	2.732	1.00	25.04
ATOM	1675	CA	GLU A	212	19.485	68.311	3.777	1.00	26.00

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						- 65 -				31.89
				212	20.580	ე 68	3.763	4.742	1.00	52.30
MOTA	1676	CB	GLU A	212 212	21.00		7.726	5.770	1.00 1.00	60.61
ATOM	1677	CG	GLU A	212	21.60		5.472	5.145	1.00	59.97
MOTA	1678	CD	GLU A GLU A	212	20.90		5.434	5.092	1.00	67.14
ATOM	1679	OE1	GLU A	212	22.78	6 66	6.527	4.718	1.00	24.80
ATOM	1680	OE2	GLU A	212	18.15	8 6	8.100	4.500 4.392	1.00	22.54
MOTA	1681	С 0	GLU A	212	17.24		8.918	5.234	1.00	26.64
MOTA	1682	И	TRP A	213	18.05	-	6.997	5.963	1.00	28.18
ATOM	1683 1684	CA	TRP A	213	16.84		6.653	6.811	1.00	27.08
ATOM	1685	СВ	TRP A	213	17.06	_	5.393 5.589	7.993	1.00	31.90
MOTA	1686	CG	TRP A	213	17.94		6.016	9.295	1.00	34.81
MOTA	1687	CD2	TRP A	213	17.5		6.070	10.093	1.00	39.48 35.14
ATOM ATOM	1688	CE2	TRP A	213	18.7		66.353	9.867	1.00	34.70
ATOM	1689	CE3	TRP A	213	16.3 19.2	••	65.406	8.051	1.00	38.91
ATOM	1690	CD1	TRP A	213	19.7		65.698	9.306	1.00 1.00	39.22
ATOM	1691	NE1	TRP A	213 213	18.6		66.456	11.436	1.00	36.20
MOTA	1692	CZ2	TRP A	213	16.2	78	66.736	11.198	1.00	39.04
ATOM	1693	CZ3	TRP A	_	17.4	52	66.780	11.969 6.840	1.00	27.32
MOTA	1694	CH2	TRP A		16.3	12	67.780	7.341	1.00	26.78
MOTA	1695	С 0	TRP A		17.0	74	68.601	7.033	1.00	25.99
MOTA	1696	И	HIS A		14.9		67.785	9.843	1:00	21.26
ATOM	1697	CA	HIS A				68.785	7.229	1.00	24.00
ATOM	1698	CB	HIS F				70.170	5.815	1.00	26.31
MOTA	1699 1700	CG	HIS A				70.268 70.964	5.265	1.00	20.40
MOTA	1701	CD2	HIS 2	A 214			69.575	4.782	1.00	24.70
ATOM	1702	NDl				604	69.840	3.657	1.00	19.84
MOTA	1703	CEI				966	70.682	3.921	1.00	19.56 20.75
ATOM ATOM	1704	NE2				.983 .824	68.508	7.915	1.00	22.27
ATOM	1705	С	HIS		·	. 295	67.628	7.230	1.00	21.29
ATOM	1706	0	HIS		_	. 153	69.316	8.718	1.00	25.72
MOTA	1707	N	GLU		<u>-</u>	.710	69.258	8.888	1.00 1.00	27.88
MOTA	1708	Q	GLU		_	.347	68.937	10.341	1.00	44.01
MOTA	1709	CB	GLU		-	.325	69.505	11.344	1.00	49.99
ATOM	1710	CG		-		.962	69.188	12.773	1.00	48.65
MOTA	1711	CD		-		.532	68.043	13.040 13.628	1.00	56.84
MOTA	1712	OE OE				118	70.089	8.504	1.00	23.84
MOTA	1713	C	GLU			.320	70.676	8.672	1.00	24.88
MOTA	1714	_	GLU			1.116	71.595	7.935	1.00	22.73
ATOM	1715 1716		ASP			9.136	70.858 72.187	7.492	1.00	22.94
MOTA	1717		A ASP	A 2		8.732	72.112	6.407	1.00	27.97
MOTA	1718	~				7.636	71.398	5.135	1.00	27.71 31.88
ATOM	1719	_			- -	8.082	71.232	4.918	1.00	26.49
ATOM ATOM	1720	_				9.304 7.185	71.015	4.344	1.00	19.73
ATOM	1721	1 0				8.230	73.096	8.596	1.00 1.00	23.16
MOTA	1723		- ~		216 216	7.680	72.652	9.594	1.00	16.59
ATOM	172	3 C		_	217	8.433	74.384	8.398	1.00	18.55
MOTA	172			_	217	7.945	75.376	9.312	1.00	16.49
MOTA	172	· .			217	8.907	76.564	9.424 10.235	1.00	10.45
MOTA	172	-		_	217	8.265	77.687	10.088	1.00	11.70
MOTA	172			LΑ	217	10.179	76.123	8.633	1.00	23.10
MOTA	172	. •		L A	217	6.652	75.819	7.729	1.00	21.60
MOTA	172 173			AL A	217	6.667	76.674 75.142	8.990	1.00	
MOTA	173			ER A	218	5.562	75.433	8.452	1.00	
ATOM	173		CA S	ER A	218	4.233	75.110	6.954	1.00	
MOTA	17		CB S	ER A	218	4.183	73.706	6.717	1.00	
ATOM ATOM	17			ER A	218	4.109 3.190	74.585	9.178	1.00	
MOTA		35	_	ER A	218	3.541	73.734	9.996	1.0	
ATOM		36	-	ER A	218	1.913	74.865	8.932		
ATOM	17	137	• •	EU A	219 219	0.847	74.064	9.518		
ATOM	17	738	٠	EU A	219	-0.493		9.483		
ATOM		739	-	LEU A	219	-1.687	73.96	9.955		
ATOM	17	740		LEU A	219	-1.427	73.41		· .	
MOTA	1.	741		LEU A	219	-2.933	74.80	0 (7)		
MOTA	1	742		LEU A	219	0.822	72.81			00 26.48
ATOM		743	-	LEU A	219	0.870	07		_	00 24.79
MOTA		744	-	ILE A	220	0.76	^/	~	_	00 22.56
ATOM	•	745	CA	ILE A	220	0.82	70		0 1.	
MOTA	•	.746 L747	CB .	ILE A	220	-0.56	70 9/	7 04		00 20.63
ATO	•	1748	CG2	ILE A		-1.33	> /0.8			
ATO	rn -									

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MOTA	- ,	49 C	G1 II	LE A	220	-1.380					
ATOM	- '	-		EA	220	-2.509		5.10	9 1.0	0 22.4	1 2
ATOM		_		ΕA	220	1.501			7 1.0		
ATOM ATOM	~ ' .			EΑ	220	1.496		_	0	0 18.5	
ATOM	179	_		RA	221	2.141		,,	4.0		
ATOM	179			R A	221	2.802				0 17.7	
ATOM	175				221	4.287		_		0 14.9	
ATOM	175				221	4.937				0 15.9	
ATOM	175				221	4.928	72.46			18.7	
ATOM	175 175				221	2.066	71.65				1
ATOM	176	-			221	1.711	70.477		+.00		0
ATOM	176				222	1.729	72.477	,	00	0	
ATOM	176:				222	0.992	72.088		-,00	-0.01	
ATOM	176.					-0.332	72.880				
ATOM	1764					-1.046	72.671	-1.630			
ATOM	1765		VAL			-1.221	72.446	0.854			
ATOM	1766		VAL	_	22	1.890	72.404	-1.464	1.00		
ATOM	1767	7 N	LEU	_	23	1.990	73.557	-1.895	1.00	17.84	
ATOM	1768	CA	LEU	_	23	2.525	71.359	-1.995	1.00	18.42 14.96	
ATOM	1769	CB	LEU	_	23	3.495	71.469	-3.080	1.00	15.97	
ATOM	1770	CG	LEU	_		4.779 5.836	70.761	-2.647	1.00	8.17	
ATOM	1771					6.771	70.407	-3.680	1.00	9.19	
ATOM	1772	CD2				6.605	71.557	-3.882	1.00	9.69	
ATOM ATOM	1773	C	LEU			3.146	69.205	-3.191	1.00	12.71	
ATOM	1774	0	LEU			2.623	70.951	-4.461	1.00	20.09	
ATOM	1775	N	TYR			3.453	69.846 71.757	-4.608	1.00	24.25	
ATOM	1776	CA	TYR			3.283	71.737	-5.476	1.00	23.92	
ATOM	1777	CB	TYR			2.415	72.269	-6.862	1.00	22.47	
ATOM	1778	CG	TYR			2.258	71.701	-7.711	1.00	25.33	
ATOM	1779 1780	CD1	TYR .		4 1	L.592	70.488	-9.110 -9.311	1.00	24.10	
ATOM	1781	CE1	TYR		_	1.534	69.893	-10.560	1.00	22.12	
ATOM	1782	CD2 CE2	TYR A			2.860	72.311	-10.212	1.00	25.03	
ATOM	1783	CZ	TYR A		_	.811	71.720	-11.475	1.00	23.73	
ATOM	1784	OH	TYR A		_	.146	70.505	-11.643	1.00	27.76	
ATOM	1785	C	TYR A		4 2	.112	69.895	-12.884	1.00	29.83	
ATOM	1786	Õ	TYR A			.680	71.314	-7.451	1.00 1.00	31.58	
ATOM	1787	N	GLN A		_	.424	72.301	-7.392	1.00	25.24	
ATOM	1788	CA	GLN A		_	.014	70.193	-8.060	1.00	27.50	
ATOM	1789	Q	GLN A			.327	70.006	-8.639	1.00	23.63	
ATOM	1790	CG	GLN A			. 184	69.294	-7.609	1.00	25.73	
ATOM	1791	CD	GLN A			.614 .378	69.292	-7.891	1.00	23.37 25.23	
ATOM	1792	OE1	GLN A	225		264	68.781	-6.720	1.00	30.69	
ATOM	1793	NE2	GLN A	225		042	69.461 67.578	-6.203	1.00	37.77	
ATOM ATOM	1794	С	GLN A	225		105	69.126	-6.278	1.00	29.82	
ATOM	1795	0	GLN A	225		503	68.056	-9.858	1.00	27.45	
ATOM	1796	N	SER A	226		601	69.552	-9.759	1.00	27.59	
ATOM	1797	CA	SER A	226		358	68.779	-11.007	1.00	27.34	
ATOM	1798 1799	CB	SER A	226	5.	501	69.605	-12.210 -13.152	1.00	28.99	
ATOM	1800	OG	SER A	226	5.	052	68.829	-14.229	1.00	28.18	
ATOM	1801	С 0	SER A	226	7.5	599	68.311	-12.943	1.00	40.16	
ATOM	1802	N	SER A	226	8.5	570	69.055	-13.087	1.00	31.56	
ATOM	1803	CA	ASN A	227	7.5		67.055	-13.370	1.00	32.05	
ATOM	1804		ASN A	227	8.6		66.471	-14.133	1.00	30.89	
ATOM	1805		ASN A ASN A	227	8.8		67.285	-15.417	1.00	29.18	
ATOM	1806		ASN A	227	9.5		66.482	-16.528	1.00 1.00	28.72	
ATOM	1807		ASN A	227	9.1		65.341	-16.779	1.00	27.74	
ATOM	1808		ASN A	227	10.4		67.089	-17.229	1.00	28.75	
ATOM	1809		ASN A	227 227	9.9		66.328	-13.380	1.00	27.94	
ATOM	1810		VAL A	228	11.0		66.517	-13.960	1.00	28.97	
ATOM	1811		VAL A	228	9.9		66.006	-12.091	1.00	30.10	
ATOM	1812		VAL A	228	11.1		65.809	-11.291	1.00	29.20	
ATOM	1813		VAL A	228	11.5 13.0		57.058	-10.497	1.00	27.27 26.29	
ATOM	1814		VAL A	228			57.241	-10.649	1.00	23.43	
ATOM	1815		/AL A	228	10.83	-	8.292	-10.859	1.00	25.97	
ATOM	1816		/AL A	228	9.65	_	4.826	-10.206	1.00	31.99	
ATOM ATOM	1817	N G	ELN A	229	11.82		64.760 64.110	-9.758	1.00	35.97	
ATOM	1818	CA G	LN A	229	11.71	_	3.153	-9.753	1.00	34.06	
ATOM	1819		LN A	229	11.79	~	1.734	-8.658	1.00	33.36	
ATOM	1820			229	11.55		0.666	-9.176	1.00	37.53	
	1821	CD G	LN A	229	11.20	_ *	9.368	-8.148 -8.833	1.00	42.23	
						_		2.0.2	1.00	55.26	

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3.0014	1822	OEl	GLN A	229	10.110	59.222	-9.392	1.00	58.46
ATOM ATOM	1823	NE2	GLN A	229	12.155	58.436	-8.857	1.00	59.25
ATOM	1824	C	GLN A	229	12.935	63.474	-7.814	1.00	34.22
ATOM	1825	ō	GLN A	229	14.044	63.042	-8.124	1.00	34.78
ATOM	1826	N	ASN A	230	12.733	64.293	-6.784	1.00	34.28
ATOM	1827	CA	ASN A	230	13.827	64.732	-5.917	1.00	32.42
ATOM	1828	C8	ASN A	230	14.171	66.199	-6.226	1.00	27.53
ATOM	1829	CG	ASN A	230	12.974	67.136	-6.068	1.00	21.96
ATOM	1830	OD1	ASN A	230	11.933	66.751	-5.545	1.00	24.46
ATOM	1831	ND2	ASN A	230	13.118	68.361	-6.541	1.00	19.87
ATOM	1832	С	ASN A	230	13.575	64.587	-4.419	1.00	31.95
ATOM	1833	0	ASN A	230	14.476	64.808	-3.622	1.00	30.47
ATOM	1834	N	LEU A	231	12.356	64.231	-4.034 -2.626	1.00 1.00	31.28 27.98
ATOM	1835	CA	LEU A	231	12.018	64.092 64.431	-2.408	1.00	24.65
ATOM	1836	CB CG	LEU A LEU A	231 231	10.551 10.254	65.884	-2.135	1.00	21.29
ATOM	1837 1838	CD1	LEU A	231	8.807	65.985	-1.745	1.00	24.61
ATOM ATOM	1839	CD2	LEU A	231	11.116	66.349	-0.993	1.00	23.04
ATOM	1840	C	LEU A	231	12.276	62.719	-2.040	1.00	30.04
ATOM	1841	0	LEU A	231	12.145	61.706	-2.725	1.00	34.74
MOTA	1842	N	GLN A	232	12.615	62.693	-0.754	1.00	30.14
MOTA	1843	CA	GLN A	232	12.834	61.4iS	-0.034	1.00	26.30
ATOM	1844	CB	GLN A	232	14.314	61.087	0.000	1.00	25.18
MOTA	1845	CG	GLN A	232	14.877	60.607	-1.315	1.00	24.42
MOTA	1846	CD	GLN A	232	16.251	59.976	-1.163	1.00	28.50
MOTA	1847	OEl	GLN A	232	17.149	60.543	-0.538	1.00	29.12
ATOM	1848	NE2	GLN A	232	16.420	58.794	-1.736	1.00	27.79
ATOM	1849	C	GLN A	232	12.313	61.614	1.392 2.015	1.00	27.21 29.07
ATOM	1850	0	GLN A	232	12.538	62.656 60.618	1.888	1.00	25.56
ATOM	1851	N CA	VAL A VAL A	233 233	11.581 11.047	60.659	3.250	1.00	23.90
ATOM ATOM	1852 1853	CB	VAL A	233	9.588	60.195	3.354	1.00	26.06
MOTA	1854	CG1	VAL A	233	8.862	61.027	4.382	1.00	28.07
ATOM	1855	CG2	VAL A	233	8.911	60.178	2.027	1.00	25.39
ATOM	1856	C	VAL A	233	11.779	59.644	4.101	1.00	27.04
ATOM	1857	0	VAL A	233	12.024	58.519	3.662	1.00	27.08
ATOM	1858	N	GLU A	234	12.090	60.015	5.331	1.00	27.08
ATOM	1859	CA	GLU A	234	12.744	59.089	6.226	1.00	28.63
ATOM	1860	CB	GLU A	234	13.512	59.848	7.289	1.00	28.65
ATOM	1861	ÇG	GLU A	234	14.044	58.977	8.400	1.00	33.81
MOTA	1862	CD	GLU A	234	14.652	59.788	9.509 9.558	1.00 1.00	37.83 46.49
ATOM	1863	OE1	GLU A	234 234	15.893	59.870 60.356	10.323	1.00	41.82
ATOM	1864	OE2 C	GLU A GLU A	234	13.894 11.637	58.292	6.881	1.00	32.99
ATOM ATOM	1865 1866	0	GLU A	234	10.761	58.861	7.526	1.00	36.86
ATOM	1867	N	THR A	235	11.619	56.990	6.654	1.00	39.05
ATOM	1868	CA	THR A	235	10.603	56.144	7.264	1.00	43.64
ATOM	1869	СВ	THR A	235	9.789	55.370	6.196	1.00	47.64
ATOM	1870	OG1	THR A	235	10.663	54.518	5.443	1.00	48.96
MOTA	1871	CG2	THR A	235	9.077	56.340	5.245	1.00	49.04
ATOM	1872	C	THR A	235	11.310	55.161	8.186	1.00	45.27
MOTA	1873	0	THR A	235	12.533	55.204	8.330	1.00	46.15
MOTA	1874	N	ALA A	236	10.549	54.266	8.802	1.00	48.85
ATOM	1875	CA	ALA A	236	11.131	53.271	9.697 10.416	1.00	51.37 52.57
ATOM	1876	CB	ALA A	236	10.035	52.506 52.3 0 7	8.944	1.00	51.92
ATOM	1877	C	ALA A	236 236	12.049 12.709	51.464	9.547	1.00	56.47
MOTA	1878	N O	ALA A ALA A	237	12.044	52.402	7.620	1.00	50.60
ATOM ATOM	1879 1880	CA	ALA A	237	12.886	51.558	6.786	1.00	50.28
ATOM	1881	CB	ALA A	237	12.044	50.870	5.720	1.00	45.48
ATOM	1882	c	ALA A	237	13.952	52.421	6.126	1.00	51.53
ATOM	1883	0	ALA A	237	14.591	51.992	5.156	1.00	53.02
ATOM	1884	N	GLY A	238	14.159	53.620	6.672	1.00	49.22
MOTA	1885	CA	GLY A	238	15.129	54.542	6.108	1.00	47.88
MOTA	1886	С	GLY A	238	14.493	55.410	5.029	1.00	46.36
ATOM	1887	0	GLY A	238	13.275	55.377	4.837	1.00	45.44
ATOM	1888	N	TYR A	239	15.305	56.193	4.325	1.00	43.94
MOTA	1889	CA	TYR A	239	14.795	57.077	3.282	1.00 1.00	42.31 34.38
MOTA	1890	CB	TYR A	239	15.860	58.079	2.862 3.846	1.00	31.86
MOTA	1891	CG	TYR A	239 239	16.054 16.902	59.203 59.064	4.943	1.00	29.03
ATOM	1892	CD1 CE1	TYR A	239	17.115	60.129	5.825	1.00	30.21
MOTA MOTA	1893 1894	CD2	TYR A	239	15.416	60.427	3.659	1.00	31.58
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ATOM	1895	CE2	TYR A	239	15.618	61.491	4.536	1.00	27.77
MOTA	1896	CZ	TYR A	239	16.467	61.337	5.609	1.00	28.27
ATOM	1897	OH	TYR A	239	16.670	62.396	6.459	1.00	30.28
ATOM	1898	С	TYR A	239	14.282	56.345	2.053	1.00	44.25
ATOM	1899	0	TYR A	239	14.958	55.464	1.519	1.00	50.07
ATOM	1900	N	GLN A	240	13.089	56.730	1.605	1.00	42.95
ATOM	1901	CA	GLN A	240	12.457	56.135	0.434	1.00	37.56
ATOM	1902	CB	GLN A	240	11.227	55.338	0.829	1.00	37.90
ATOM ATOM	1903 1904	CG CD	GLN A GLN A	240 240	11.492 10.259	54.283 53.503	1.867 2.178	1.00	39.00
ATOM	1905	OE1	GLN A	240	9.361	53.975	2.876	1.00	41.54 42.44
ATOM	1906	NE2	GLN A	240	10.192	52.303	1.655	1.00	43.71
ATOM	1907	С	GLN A	240	12.036	57.238	-0.493	1.00	35.12
ATOM	1908	0	GLN A	240	11.637	58.310	-0.049	1.00	37.16
ATOM	1909	N	ASP A	241	12.106	56.963	-1.786	1.00	37.65
ATOM	1910	CA	ASP A	241	11.757	57.937	-2.807	1.00	33.97
ATOM	1911	CB	ASP A	241	12.294	57.477	-4.157	1.00	36.71
ATOM	1912	CG	ASP A	241	13.768	57. 72 5	-4.305	1.00	40.53
ATOM	1913	OD1	ASP A	241	14.501	56.767	-4.626	1.00	48.07
ATOM ATOM	1914 191S	OD2 C	ASP A ASP A	241 241	14.193 10.273	58.883 58.187	-4.102 -2.937	1.00	43.60
ATOM	1916	0	ASP A	241	9.473	57.290	-2.715	1.00 1.00	31.87 33.89
ATOM	1917	N	ILE A	242	9.910	59.420	-3.270	1.00	29.50
MOTA	1918	CA	ILE A	242	8.516	59.776	-3.491	1.00	29.59
MOTA	1919	CB	ILE A	242	8.122	61.110	-2.793	1.00	25.82
ATOM	1920	CG2	ILE A	242	6.718	61.540	~3.205	1.00	21.57
ATOM	1921	CG1	ILE A	242	8.142	60.940	-1.275	1.00	22.34
ATOM	1922	CD1	ILE A	242	7.931	62.219	-0.529	1.00	19.47
ATOM	1923	С	ILE A	242	8.314	59.899	-5.002	1.00	32.14
ATOM	1924	0	ILE-A	242	9.039	60.631	-5.680	1.00	34.26
ATOM ATOM	1925 1926	N CA	GLU A GLU A	243 243	7.364 7.051	59.139	-5.528	1.00	32.42
ATOM	1927	CB	GLU A	243	5.998	59.161 58.103	-6.950 -7.257	1.00	35.87 45.32
ATOM	1928	CG	GLU A	243	4.620	58.422	-6.675	1.00	58.52
ATOM	1929	CD	GLU A	243	3.584	57.359	-6.970	1.00	67.74
ATOM	1930	OE1	GLU A	243	2.679	57.157	-6.126	1.00	72.36
ATOM	1931	OE2	GLU A	243	3.669	56.730	-8.048	1.00	73.67
ATOM	1932	С	GLU A	243	6.494	60.520	-7.361	1.00	34.26
ATOM	1933	0	GLU A	243	5.794	61.170	-6.587	1.00	34.70
ATOM	1934	N	ALA A	244	6.796	60.940	-8.582	1.00	37.14
ATOM	1935	CA	ALA A	244	6.299	62.211	-9.106	1.00	36.70
ATOM ATOM	1936 19 3 7	CB C	ALA A ALA A	244 244	7.187 4.870	62.704 62.045	-10.237	1.00	30.95
ATOM	1937	0	ALA A	244	4.401	60.919	-9.607 -9.809	1.00	38.29 39.49
ATOM	1939	N	ASP A	245	4.184	63.168	-9.810	1.00	38.94
MOTA	1940	CA	ASP A	245	2.809	63.171	-10.302	1.00	36.20
ATOM	1941	CB	ASP A	245	1.849	62.683	-9.217	1.00	35.69
ATOM	1942	CG	ASP A	245	0.436	62.479	-9.730	1.00	39.12
ATOM	1943	OD1	ASP A	245	-0.090	63.350	-10.446	1.00	38.32
MOTA	1944	OD2	ASP A	245	-0.162	61.440	-9.406	1.00	44.34
ATOM	1945	C	ASP A	245	2.423	64.579	-10.720	1.00	36.64
ATOM	1946	0	ASP A	245	1.881	65.338	-9.920	1.00	40.34
MOTA MOTA	1947 1948	N CA	ASP A ASP A	246 246	2.624 2.288	64.906 66.242	-11.989 -12.464	1.00	36.70
ATOM	1949	C8	ASP A	246	2.956	66.546	-13.815	1.00 1.00	42.59 52.74
ATOM	1950	CG	ASP A	246	2.651	65.508	-14.899	1.00	62.16
MOTA	1951	OD1	ASP A	246	3.484	65.398	-15.834	1.00	67.79
ATOM	1952	OD2	ASP A	246	1.600	64.822	-14.836	1.00	61.80
ATOM	1953	C	ASP A	246	0.818	66.649	-12.495	1.00	39.27
MOTA	1954	0	ASP A	246	0.485	67.699	-13.042	1.00	39.09
MOTA	1955	N	THR A	247	-0.058	65.849	-11.897	1.00	37.20
MOTA	1956	CA	THR A	247	-1.479	66.182	-11.876	1.00	37.88
ATOM	1957	CB	THR A	247	-2.345	65.074	-12.545	1.00	41.31
ATOM	1958	OG1	THR A	247	-2.370 -3.770	63.901	-11.719	1.00	44.54
ATOM ATOM	1959 1960	CG2 C	THR A	247 247	-1.770 -1.990	64.688 66.436	-13.903 -10.452	1.00 1.00	42.77 37.12
ATOM	1960	0	THR A	247	-3.109	66.933	-10.452	1.00	37.12
ATOM	1962	N	GLY A	248	-1.162	66.136	-9.453	1.00	33.34
ATOM	1963	CA	GLY A	248	-1.580	66.320	-8.076	1.00	29.08
ATOM	1964	C	GLY A	248	-0.704	67.236	-7.251	1.00	26.86
ATOM	1965	0 .	GLY A	248	0.338	67.693	-7.709	1.00	29.61
ATOM	1966	N	TYR A	249	-1.168	67.553	-6.052	1.00	24.24
ATOM	1967	CA	TYR A	249	-0.432	68.401	-5.128	1.00	22.26

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	1968	СВ	TYR A	249	-1.319	69.512	-4.571	1.00	17.04
ATOM ATOM	1969	CG			-1.337	70.775	-5.395	1.00	19.97
ATOM	1970	CD1		249	-2.159	70.896	-6.505	1.00	21.32
ATOM	1971	CEl	TYR A		-2.194	72.078	-7.247	1.00	22.14 17.14
ATOM	1972	CD2			-0.545	71.866	-5.045 -5.777	1.00 1.00	18.05
MOTA	1973	CE2			-0.575	73.041	-6.876	1.00	18.13
MOTA	1974	CZ			-1.398	73.140 74.302	-7.612	1.00	23.74
MOTA	1975	ОН		249 249	0.037	67.520	-3.982	1.00	24.44
ATOM	1976	C 0	TYR A	249	-0.766	66.320	-3.363	1.00	25.35
ATOM	1977 1978	И	LEU A	250	1.344	67.505	-3.745	1.00	21.09
MOTA MOTA	1979	CA	LEU A	250	1.908	66.720	-2.664	1.00	19.72
ATOM	1980	CB	LEU A	250	3.397	66.484	-2.914	1.00	11.66
MOTA	1981	CG	LEU A	250	4.092	65.533	-1.946	1.00	13.51 9.39
ATOM	1982	CD1	LEU A	250	3.460	64.158	-1.998 -2.310	1.00	16.26
ATOM	1983	CD2	LEU A	250	5.536	65.450 67.475	-1.349	1.00	24.50
MOTA	1984	C	LEU A	250 250	1.683 2.160	68.606	-1.176	1.00	23.74
ATOM	1985	O N	LEU A ILE A	251	0.953	66.847	-0.432	1.00	25.00
ATOM	1986 1987	CA	ILE A	251	0.651	67.447	0.866	1.00	23.54
ATOM ATOM	1988	CB	ILE A	251	-0.876	67.411	1.138	,1.00	21.64
ATOM	1989	CG2	ILE A	251	-1.257	68.522	2.121	1.00	20.73
ATOM	1990	CG1	ILE A	251	-1.670	67.562	-0.169	1.00	18.11
ATOM	1991	CD1	ILE A	251	-1.594	68.929	-0.792	1.00	15.82 25.96
ATOM	1992	С	ILE A	251	1.376	66.775	2.071 2.148	1.00	22.81
MOTA	1993	0	ILE A	251	1.478	65.545 67.590	2.979	1.00	27.93
ATOM	1994	N	ASN A	252 252	1.919 2.583	67.097	4.190	1.00	23.28
ATOM	1998	CA	ASN A ASN A	252	4.067	66.731	3.969	1.00	19.24
ATOM	1996 1997	CB CG	ASN A	252	4.949	67.922	3.669	1.00	15.95
ATOM ATOM	1998	OD1	ASN A	252	5.210	68.225	2.521	1.00	27.71
MOTA	1999	ND2	ASN A	252	5.482	68.544	4.698	1.00	12.20
ATOM	2000	С	ASN A	252	2.417	68.107	5.321	1.00	26.77
MOTA	2001	0	ASN A	252	2.046	69.258	5.079	1.00 1.00	26.57 26.39
ATOM	2002	N	CYS A	253	2.621	67.649	6.555 7.744	1.00	23.80
MOTA	2003	CA	CYS A	253	2.484	68.488 67.638	8.950	1.00	26.15
MOTA	2004	CB	CYS A	253	2.069 0.326	67.176	9.038	1.00	32.10
MOTA	2005	SG	CYS A CYS A	253 253	3.758	69.222	8.107	1.00	20.68
ATOM	2006 2007	C 0	CYS A	253	4.853	68.766	7.810	1.00	23.52
MOTA MOTA	2008	N	GLY A	254	3.601	70.371	8.740	1.00	21.10
ATOM	2009	CA	GLY A	254	4.740	71.143	9.183	1.00	21.44
ATOM	2010	С	GLY A	254	4.870	70.886	10.669	1.00	19.86 17.78
ATOM	2011	0	GLY A	254	4.062	70.173	11.245 11.325	1.00 1.00	21.03
MOTA	2012	N	SER A	255	5.839	71.492 71.237	12.737	1.00	20.86
MOTA	2013	CA	SER A	255 255	5.996 7.348	71.742	13.225	1.00	16.65
MOTA	2014	CB	SER A SER A	255	7.529	73.096	12.870	1.00	24.84
MOTA	2015	OG C	SER A	255	4.862	71.800	13.592	1.00	25.80
MOTA MOTA	2016 2017	0	SER A	255	4.635	71.316	14.702	1.00	32.81
ATOM	2018	N	TYR A	256	4.132	72.800	13.103	1.00	23.31
ATOM	2019	CA	TYR A	256	3.048	73.337	13.916	1.00 1.00	22.05 18.59
MOTA	2020	CB	TYR A	256	2.453	74.597	13.320 14.313	1.00	18.81
ATOM	2021	CG	TYR A	256	1.600	75.359 76.147	15.301	1.00	14.81
ATOM	2022	CD1	TYR A	256	2.181 1.399	76.878	16.198	1.00	18.34
MOTA	2023	CE1	TYR A TYR A	256 256	0.213	75.302	14.253	1.00	22.82
MOTA	2024	CD2 CE2	TYR A	256	-0.586	76.029	15.151	1.00	22.41
MOTA MOTA	2025 2026	CZ	TYR A	256	0.015	76.812	16.122	1.00	22.48
ATOM	2027	ОН	TYR A	256	-0.777	77.531	16.994	1.00	27.35
ATOM	2028	С	TYR A	256	1.946	72.303	14.160	1.00	25.24 30.73
ATOM	2029	0	TYR A	256	1.377	72.250	15.249	1.00	25.21
ATOM	2030	N	MET A	257	1.645	71.490	13.152 13.281	1.00	25.59
MOTA	2031	CA	MET A	257	0.633	70.443 69.749	11.930	1.00	23.11
MOTA	2032	CB	MET A	257 257	0.422 -0.631	68.646	11.889	1.00	23.77
MOTA	2033	CG	MET A	257	-2.303	69.226	12.196	1.00	29.13
ATOM	2034	SD CE	MET A		-2.926	69.464	10.571	1.00	21.14
ATOM	2035 2036	C	MET A		1.118	69.444	14.338	1.00	29.65
ATOM ATOM	2037	o	MET A		0.348	68.996	15.182	1.00	33.68
ATOM	2038	N	ALA A	258	2.410	69.139	14.324	1.00	30.20 29.21
ATOM	2039	CA	ALA A		2.975	68.207	15.294 14.962	1.00 1.00	26.53
ATOM	2040	СВ	ALA A	258	4.437	67.918	14.302	1.00	_0.53

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MOTA	2041	С	ALA A	258	2.843	68.740	16.721	1.00	29.82
ATOM	2042	0	ALA A	258	2.486	67.999	17.635	1.00	30.07
ATOM	2043	N	HIS A	259	3.130	70.023	16.912	1.00	29.81
ATOM ATOM	2044 2045	CA CB	HIS A HIS A	259	3.023	70.635	18.231	1.00	30.03
ATOM	2046	CG	HIS A	259 259	3.560 3.2 7 9	72.061 72.846	18.197	1.00	29.44
ATOM	2047	CD2	HIS A	259	3.973	72.846	19.441 20.600	1.00	36.67
ATOM	2048	ND1	HIS A	259	2.174	73.662	19.572	1.00	35.37 39.99
ATOM	2049	CE1	HIS A	259	2.201	74.255	20.750	1.00	40.19
ATOM	2050	NE2	HIS A	259	3.284	73.854	21.397	1.00	33.91
ATOM	2051	C	HIS A	259	1.571	70.645	18.703	1.00	32.65
ATOM ATOM	2052 2053	O N	HIS A	259	1.295	70.499	19.884	1.00	37.28
MOTA	2054	CA	LEU A LEU A	260 260	0.650 -0.770	70.862 70.900	17.778 18.092	1.00	33.08
MOTA	2055	СВ	LEU A	260	-1.543	71.402	16.880	1.00	31.90
ATOM	2056	CG	LEU A	260	-2.224	72.751	16.957	1.00	30.79 33.95
ATOM	2057	CD1	LEU A	260	-1.342	73.763	17.664	1.00	35.15
ATOM	2058	CD2	LEU A	260	-2.549	73.184	15.536	1.00	39.19
ATOM ATOM	2059 2060	C	LEU A	260	-1.326	69.536	18.470	1.00	33.38
ATOM	2061	O N	LEU A THR A	260 261	-2.082 -0.988	69.411	19.420	1.00	35.86
ATOM	2062	CA	THR A	261	-1.480	68.526 67.184	17.684 17.905	1.00	32.53
ATOM	2063	CB	THR A	261	-1.571	66.443	16.580	1.00	33.81 35.83
ATOM	2064	OG1	THR A	261	-0.270	66.392	15.977	1.00	33.48
ATOM	2065	CG2	THR A	261	-2.537	67.155	15.647	1.00	37.64
ATOM	2066	С	THR A	261	-0.590	66.389	18.840	1.00	39.46
ATOM ATOM	2067 2068	O N	THR A ASN A	261 262	-0.651	65.153	18.870	1.00	38.94
ATOM	2069	CA	ASN A	262	0.267 1.191	67.094 66.456	19.572 20.506	1.00	44.19
ATOM	2070	CB	ASN A	262	0.445	65.952	21.756	1.00	49.58 59.13
ATOM	2071	CG	ASN A	262	1.353	65.841	22.981	1.00	66.86
MOTA	2072	OD1	ASN A	262	1.367	66.737	23.833	1.00	72.04
MOTA	2073	ND2	ASN A	262	2.105	64.743	23.081	1.00	67.84
ATOM ATOM	2074 2075	С 0	ASN A ASN A	262	1.941	65.307	19.811	1.00	46.90
ATOM	2076	И	ASN A	262 263	2.228 2.208	64.274 65.492	20.415 18.522	1.00	49.43
ATOM	2077	CA	ASN A	263	2.929	64.534	17.698	1.00 1.00	41.44 37.52
ATOM	2078	C13	ASN A	263	4.237	64.119	18.347	1.00	41.11
ATOM	2079	CG	ASN A	263	5.415	64.740	17.670	1.00	47.69
ATOM	2080	OD1	ASN A	263	5.928	65.764	18.109	1.00	48.68
ATOM ATOM	2081 2082	ND2 C	ASN A ASN A	263	5.824	64.155	16.550	1.00	54.33
ATOM	2083	0	ASN A	263 263	2.201 2.832	63.322 62.388	17.172	1.00	35.18
ATOM	2084	N	TYR A	264	0.877	63.344	16.679 17.250	1.00 1.00	34.27 36.95
MOTA	2085	CA	TYR A	264	0.063	62.252	16.723	1.00	37.39
TOM	2086	CB	TYR A	264	-1.393	62.413	17.189	1.00	33.82
ATOM ATOM	2087	CG	TYR A	264	-2.344	61.342	16.713	1.00	33.63
ATOM	2088 2089	CD1 CE1	TYR A TYR A	264 264	-2.446	60.113	17.362	1.00	32.49
ATOM	2090	CD2	TYR A	264	-3.375 -3.180	59.t S1 61.5 7 9	16.935 15.627	1.00	33.06
ATOM	2091	CE2	TYR A	264	-4.105	60.636	15.195	1.00 1.00	37.61 37.45
ATOM	2092	CZ	TYR A	264	-4.204	59.429	15.845	1.00	35.62
ATOM	2093	ОН	TYR A	264	-5.169	58.546	15.403	1.00	38.87
ATOM	2094	C	TYR A	264	0.218	62.311	15.186	1.00	37.01
ATOM ATOM	2095 2096	O N	TYR A TYR A	264 265	0.169 0.390	61.287	14.499	1.00	37.37
ATOM	2097	CA	TYR A	265	0.642	63.528 63.768	14.666 13.244	1.00 1.00	36.23
ATOM	2098	CB	TYR A	265	-0.351	64.750	12.640	1.00	33.20 26.57
ATOM	2099	CG	TYR A	265	-1.642	64.115	12.239	1.00	31.72
ATOM	2100	CD1	TYR A	265	-2.630	64.861	11.610	1.00	33.04
ATOM ATOM	2101	CE1	TYR A	265	-3.854	64.298	11.286	1.00	30.94
ATOM	2102 2103	CD2 CE2	TYR A TYR A	265 265	-1.909	62.775	12.527	1.00	32.98
ATOM	2103	CZ	TYR A	265	-3.141 -4.102	62.201 62.976	12.207 11.591	1.00	31.76
ATOM	2105	ОН	TYR A	265	-5.333	62.452	11.312	1.00	30.37 38.15
ATOM	2106	C	TYR A	265	2.028	64.390	13.227	1.00	34.58
ATOM	2107	0	TYR A	265	2.187	65.586	13.466	1.00	35.29
ATOM ATOM	2108	N C2	LYS A	266	3.036	63.553	13.022	1.00	34.31
ATOM	·2109 2110	CA CB	LYS A LYS A	266 266	4.422 5.328	63.990	13.002	1.00	33.62
ATOM	2111	CG	LYS A	266	6.739	62.772 63.066	13.039 13.491	1.00 1.00	39.20
ATOM	2112	CD	LYS A	266	7.549	61.773	13.584	1.00	56.22 67.11
ATOM	2113	CE	LYS A	266	6.797	60.697	14.372	1.00	74.71

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						15.748	1.00	80.37
	2114		S A 266	6.402	61.147	11.759	1.00	29.29
MOTA	2115	C LY	S A 266	4.748	64.784	10.702	1.00	30.14
MOTA	2116		S A 266	4.184	64.540	11.890	1.00	26.90
ATOM	2117		A A Z67	5.641	65.752	10.735	1.00	27.00
ATOM	2118		A A 267	6.063	66.526	11.173	1.00	22.67
MOTA	2119		LA A 267	6.724	67.809	10.072	1.00	28.13
MOTA	2120		LA A 267	7.079	65.599	10.695	1.00	31.38
MOTA	2121		LA A 267	8.074	65.243	8.823	1.00	30.02
MOTA	2122		RO A 268	6.822	65.155	7.989	1.00	29.53
ATOM	2123		RO A 268	5.648	65.466	8.103	1.00	28.12
ATOM	2124		RO A 268	7.732	64.251	6.742	1.00	25.57
ATOM	2125	-	RO A 268		64.081	7.035	1.00	25.50
MOTA	2125		RO A 268	5.615	64.286	7.904	1.00	27.55
MOTA	2127		RO A 268		64.805	7.555	1.00	31,71
ATOM	2128		RO A 268		65.974	8.156	1.00	26.79
MOTA	2129		LE A 269		63.984	7.939	1.00	21.70
ATOM	2130		LE A 269		64.374	8.799	1.00	23.68
ATOM	2131		LE A 269	12.527	63.535	8.358	1.00	16.90
MOTA	2132		LE A 269		63.768	10.286	1.00	25.36
MOTA	2132		ILE A 269		63.881	10.235	1.00	21.95
ATOM	2134		ILE A 269	9 12.761	65.311	6.470	1.00	21.77
MOTA	2135		ILE A 26	9 11.788	64.052	6.025	1.00	23.31
MOTA		-	ILE A 26	9 11.544	62.932		1.00	22.73
MOTA	2136		HIS A 27	0 12.196	65.043	5.696	1.00	21.55
MOTA	2137	-	HIS A 27	0 12.420	64.808	4.280	1.00	20.47
ATOM	2138		HIS A 27	0 11.161	65.146	3.480	1.00	16.63
MOTA	2139		HIS A 27	0 10.613	66.507	3.758	1.00	20.91
ATOM	2140		HIS A 27	0 10.417	67.570	2.946	1.00	18.74
ATOM	2141		HIS A 27	0 10.148	66.885	4.997	1.00	20.88
MOTA	2142	CEl	HIS A 27	9.680	68 .117	4.936	1.00	17.58
MOTA	2143	NE2	HIS A 27	9.828	68.559	3.700	1.00	22.67
MOTA	2144	C	HIS A 27		65.600	3.783	1.00	23.83
ATOM	2145	0	HIS A 2		66.588	4.410	1.00	20.85
ATOM	2146	N		71 14.201	65.136	2.689	1.00	23.79
MOTA	2147			71 15.359	65.797	2.093	1.00	22.83
MOTA	2148	CA		71 16.631	65.043	2.461	1.00	23.45
MOTA	2149	CB		71 16.615	63.592	2.057		25.22
ATOM	2150	CG		71 17.872	62.894	2.523	1.00 1.00	26.89
MOTA	2151	CD		71 18.020	61.603	1.862	1.00	25.53
MOTA	2152	NE		71 19.008	60.753	2.103		29.48
MOTA	2153	CZ		71 19.931	61.058	2.996	1.00	25.73
MOTA	2154	NH1		71 19.081	59.607	1.441	1.00	23.68
ATOM	2155	NH2		71 15.190	65.873	0.580	1.00	26.81
· ATOM	2156	C		71 14.319	65.211	0.010	1.00	22.19
MOTA	2157	0		72 15.994	66.702	-0.071	1.00	18.76
MOTA	2158	N		15.878	66.857	-1.510	1.00	17.63
MOTA	2159	Q		272 15.561	68.310	-1.870	1.00	18.50
MOTA	2160	CB		272 15.326	68.446	-3.355	1.00	15.11
ATOM	2161	CG1		272 14.340		-1.107	1.00	25.28
MOTA	2162	CG2		272 17.132		-2.248	1.00	29.40
MOTA	2163	С		272 18.202		-2.050	1.00	27.72
ATOM	2164	0		273 16.985	000	-3.092	1.00	25.89
ATOM	2165	N		273 18:059		-3.919	1.00	27.95
ATOM	2166	CA		273 17.572		-4.645	1.00	
ATOM	2167	CB	LYS A			-3.753	1.00	31.66
MOTA	2168	CG	LYS A			-4.376	1.00	35.66
MOTA	2169	CD	LYS A			-5.621	1.00	41.21
ATOM	2170	CE	LYS A			-5.974	1.00	42.41
MOTA	2171		LYS A			-4.968	1.00	25.96
MOTA	2172	С.	LYS A			-5.486	1.00	26.05
ATOM	2173	0	LYS A			-5.268	1.00	25.99
MOTA	2174	N	TRP A			-6.267	1.00	24.01
ATOM	2175	Q	TRP A	274 20.45		-6.096	1.00	24.20
MOTA	2176		TRP A	274 21.97		-7.187	1.00	23.66
ATOM	2177		TRP A	274 22.70		-8.194	1.00	21.71
MOTA	2178			274 23.52			1.00	21.28
	2179	_	TRP A	274 23.99	· ·		1.00	25.08
MOTA	2180		TRP A	274 23.90			1.00	26.21
ATOM	218			274 22.7			1.00	28.27
ATOM	218			274 23.4			1.00	
MOTA	218			274 24.8			1.00	29.23
ATOM	218		3 TRP A	274 24.7			1.00	
MOTA	218		TRP A	274 25.1			1.00	
ATOM	218	· _	TRP A	274 20.1	05 66.099	,		
ATOM	2-0							

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ATOM	218	7 0	TRP	A 27					
ATOM	218	_						1.00	32.63
ATOM	2189						-8.461	1.00	28.27
ATOM	2190						-9.825	1.00	
ATOM	2191		I VAL				-9.971	1.00	25.56
ATOM	2192		G2 VAL			66.358	~11.410	1.00	23.27
ATOM	2193		VAL VAL			65.545	-9.073	1.00	23.05
ATOM	2194					67.760	-10.689	1.00	25.58
ATOM	2195	-	VAL .	-		68.884	-10.573	1.00	23.04
ATOM	2196		ASN A			67.480	-11.532		27.65
ATOM	2197					68.539	-12.372	1.00	24.79
ATOM	2198					68.262	-12.737	1.00	23.43
ATOM	2199				23.237	69.374	-13.563	1.00	23.64
ATOM					22.697	70.479	-13.650	1.00	27.31
ATOM	2200	ND:			24.382	69.096	-14.156	1.00	25.48
ATOM	2201	C	ASN A		20.347	68.732	-13.632	1.00	32.14
ATOM	2202	0	ASN A		20.683	68.215	-14.694	1.00	24.63
ATOM	2203	N	ALA A		19.244	69.453		1.00	31.02
ATOM	2204	CA	ALA A		18.364	69.719	-13.499	1.00	25.78
	2205	CB	ALA A	277	17.502	68.507	-14.620	1.00	23.03
ATOM	2206	C	ALA A	277	17.490	70.903	-14.911	1.00	26.09
ATOM	2207	0	ALA A	277	17.232	71.177	-14.288	1.00	25.78
ATOM	2208	N	GLU A		17.034	71.602	-13.119	1.00	27.01
ATOM	2209	CA	GLU A	278	16.176		-15.321	1.00	25.92
ATOM	2210	CB	GLU A	278	16.111	72.760	-15.139	1.00	27.97
ATOM	2211	CG	GLU A	278	17.326	73.616	-16.399	1.00	29.38
ATOM	2212	CD	GLU A	278	17.328	74.473	-16.634	1.00	34.40
ATOM	2213	OE1		278	16.312	75.697	-15.764	1.00	31.39
ATOM	2214	OE2	GLU A	278		76.182	-15.327	1.00	35.93
ATOM	2215	C	GLU A	278	18.489	76.186	-15.537	1.00	37.93
ATOM	2216	0	GLU A	278	14.777	72.323	-14.767	1.00	30.01
ATOM	2217	N	ARG A	279	13.999	71.867	-15.601	1.00	33.28
ATOM	2218	CA	ARG A		14.485	72.419	-13.487	1.00	30.78
ATOM	2219	CB	ARG A	279	13.185	72.069	-12.986	1.00	29.39
ATOM	2220	CG	ARG A	279	13.232	70.718	-12.294	1.00	29.88
ATOM	2221	CD	ARG A	279	13.756	69.606	-13.168	1.00	29.15
ATOM	2222	NE		279	12.891	69.382	-14.381	1.00	
ATOM	2223	cz	ARG A ARG A	279	13.340	68.183	-15.073	1.00	26.70
ATOM	2224	NH1		279	13.978	68.185	-16.234	1.00	28.42
ATOM	2225	NH2	ARG A	279	14.224	69.324	-16.855	1.00	25.05
ATOM	2226		ARG A	279	14.477	67.059	-16.716	1.00	21.11
ATOM	2227	c	ARG A	279	12.813	73.163	-12.007	1.00	26.84
ATOM	2228	0	ARG A	279	13.645	74.001	-11.643		30.45
ATOM	2228	N	GLN A	280	11.560	73.147	-11.583	1.00	28.64
ATOM		CA	GLN A	280	11.045	74.134	-10.661	1.00	31.12
ATOM	2230	CB	GLN A	280	10.260	75.182	-11.427	1.00	33.15
ATOM	2231	CG	GLN A	280	9.171	74.580	-12.286	1.00	38.18
ATOM	2232	CD	GLN A	280	8.596	75.565	-13.278	1.00	53.46
ATOM	2233	OE1	GLN A	280	9.209	76.593	-13.568	1.00	57.41
ATOM	2234	NE2	GLN A	280	7.418	75.250		1.00	60.52
	2235	С	GLN A	280	10.138	73.430	-13.820	1.00	60.10
ATOM	2236	0	GLN A	280	9.602	72.363	-9.679	1.00	30.33
ATOM	2237	N	SER A	281	9.958	74.049	-9.975	1.00	32.02
ATOM	2238	CA	SER A	281	9.131	73.510	-8.521	1.00	26.28
ATOM	2239	CB	SER A		10.034	72.908	-7.462	1.00	18.83
ATOM	2240	OG	SER A	281	9.281		-6.390	1.00	16.21
ATOM	2241	C	SER A	281	8.344	72.175	-5.458	1.00	31.28
ATOM	2242	0	SER A	281	8.870	74.691	-6.918	1.00	17.91
ATOM	2243	N		282	7.070	75.796	-6.852	1.00	15.21
MOTA	2244	CA		282	6.239	74.487	-6.596	1.00	24.14
ATOM	2245	CB		282	5.224	75.578	-6.068	1.00	24.06
ATOM	2246	CG .		282	5.733	76.049	-7.098	1.00	26.03
ATOM	2247	CD1				76.662	-8.388	1.00	34.69
ATOM	2248	CD2			6.212	75.564	-9.339	1.00	37.28
ATOM	2249	c			4.582	77.421	-9.009	1.00	38.00
ATOM	2250	ō			5.480	75.182	-4.814	1.00	23.88
ATOM	2251	N			4.368	74.652	-4.894	1.00	21.16
ATOM	2252	CD			6.109	75.372	-3.637	1.00	
ATOM	2253	CA			7.531	75.682	-3.434	1.00	22.81
ATOM	2254	CB			5.463	75.035	-2.372	1.00	22.38
ATOM	2255	CG			6.661	74.739	-1.472	1.00	20.82
ATOM	2256			_	7.663	75.746	-1.928	1.00	18.71
ATOM	2257	C			4.651	76.192	-1.847	1.00	19.17
ATOM	2257	0 .				77.349	-2.001		17.56
ATOM		N				75.874	-1.282	1.00	19.99
	2259	CA	PHE A 2	84		76.869	-0.686	1.00	18.04
								1.00	14.83

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ATOM	2260	CB	PHE A	284	1.202	76.739	-1.221	1.00	13.11
ATOM	2261	CG	PHE A		0.222	77.695	-0.590	1.00	9.51
ATOM ATOM	2262	CD1			0.361	79.072	-0.757	1.00	7.91
ATOM	2263 2264	CD2			-0.840	77.218	0.176	1.00	8.25
ATOM	2265	CE1 CE2	PHE A PHE A		-0.546	79.963	-0.172	1.00	9.04
ATOM	2266	CZ	PHE A		-1.755 -1.607	78.103	0.769	1.00	7.90
ATOM	2267	C	PHE A	284	2.657	79.480 76.481	0.596	1.00	7.48
MOTA	2268	0	PHE A	284	2.315	75.351	0.777 1.126	1.00	15.38
MOTA	2269	N	PHE A	285	3.130	77.381	1.625	1.00	13.28
ATOM	2270	CA	PHE A	285	3.204	77.096	3.045	1.00	11.26 11.08
ATOM	2271	CB	PHE A	285	4.488	77.682	3.622	1.00	11.00
ATOM	2272	CG	PHE A	285	5.734	77.103	3.021	1.00	13.37
ATOM ATOM	2273 22 7 4	CD1	PHE A	285	6.418	77.779	2.024	1.00	12.80
ATOM	2275	CD2	PHE A PHE A	285	6.229	75.882	3.458	1.00	14.08
ATOM	2276	CE3	PHE A	285 285	7.584 7.396	77.245 75.347	1.477	1.00	16.30
MOTA	2277	CZ	PHE A	285	8.066	76.030	2.911	1.00	13.47
ATOM	2278	С	PHE A	285	1.985	77.644	1.925 3.756	1.00 1.00	7.59
ATOM	2279	0	PHE A	285	1.781	78.863	3.801	1.00	12.95 14.08
ATOM	2280	N	VAL A	286	1.150	76. 7 46	4.271	1.00	11.34
ATOM	2281	CA	VAL A	266	-0.062	77.158	4.969	1.00	15.20
ATOM ATOM	2282	CB	VAL A	286	-1.128	76.021	4.997	1.00	13.61
ATOM	2283	CG1	VAL A	286	-2.365	76.467	5.739	1.00	11.57
ATOM	2284 2285	CG2 C	VAL A VAL A	286	-1.511	75.629	3.587	1.00	10.57
ATOM	2286	0	VAL A	286 286	0.271 0.667	77.647	6.384	1.00	18.76
ATOM	2287	N	ASN A	287	0.007	76.876 78.955	7.257	1.00	24.10
ATOM	2288	CA	ASN A	287	0.461	79.568	6.571 7.850	1.00	17.87
ATOM	2289	CB	ASN A	287	1.570	80.621	7.722	1.00	18.13
ATOM	2290	CG	ASN A	287	2.940	80.017	7.427	1.00	19.63 17.67
ATOM	2291	OD1	ASN A	287	3.287	78.940	7.907	1.00	15.97
ATOM ATOM	2292	ND2	ASN A	287	3.729	80.727	6.644	1.00	19.12
ATOM	2293 2294	C O	ASN A	287	-0.844	80.242	8.229	1.00	21.86
ATOM	2295	и	ASN A LEU A	287 288	-1.584	80.680	7.347	1.00	26.85
ATOM	2296	CA	LEU A	288	~1.148 ~2.374	80.302	9.523	1.00	19.51
ATOM	2297	CB	LEU A	288	-2.853	80.928 80.254	9.979 11.253	1.00	14.83
ATOM	2298	CG	LEU A	288	-2.982	78.741	11.075	1.00	12.62
ATOM	2299	CD1	LEU A	288	-3.540	78.114	12.332	1.00	17.68 16.20
ATOM	2300	CD2	LEU A	288	-3.883	78.428	9.909	1.00	14.63
ATOM	2301	C	LEU A	288	-2.139	82.414	10.188	1.00	16.91
ATOM ATOM	2302	0	LEU A	288	-1.218	82.981	9.611	1.00	20.51
ATOM	2303 2304	N CA	GLY A GLY A	289	-2.974	83.051	10.996	1.00	16.67
ATOM	2305	C	GLY A	289 289	-2.823 -1.831	84.473	11.240	1.00	15.37
MOTA	2306	ō	GLY A	289	-1.571	84.700 83.795	12.350	1.00	19.82
ATOM	2307	N	TYR A	290	-1.342	85.924	13.130 12.477	1.00 1.00	22.79
ATOM	2308	CA	TYR A	290	-0.354	86.246	13.491	1.00	19.69 23.55
ATOM	2309	CB	TYR A	290	0.058	87.705	13.359	1.00	22.89
ATOM	2310	CG	TYR A	290	1.265	88.073	14.184	1.00	30.95
ATOM ATOM	2311	CD1	TYR A	290	2.558	87.793	13.730	1.00	31.65
ATOM	2312 2313	CE1 CD2	TYR A TYR A	290	3.671	88.142	14.481	1.00	32.74
ATOM	2313	CE2	TYR A	290 290	1.122	88.710	15.414	1.00	29.60
ATOM	2315	cz	TYR A	290	2.228 3.494	89.063 88.778	16.172	1.00	31.69
ATOM	2316	OH	TYR A	290	4.587	89.149	15.699 16.435	1.00	32.60
ATOM	2317	С	TYR A	290	-0.825	85.973	14.912	1.00 1.00	38.35 28.88
MOTA	2318	0	TYR A	290	-0.064	85.469	15.747	1.00	32.22
ATOM	2319	N	ASP A	291	-2.080	86.302	15.180	1.00	32.16
ATOM	2320	CA	ASP A	291	-2.650	86.121	16.505	1.00	34.89
ATOM ATOM	2321	CB	ASP A	291	-3.621	87.271	16.809	1.00	44.67
ATOM	2322 2323	CG OD1	ASP A ASP A	291 291	-2.907	88.607	17.064	1.00	54.47
ATOM	2323	OD1	ASP A	291	-1.678 -3.583	88.612	17.294	1.00	62.50
ATOM	2325	C	ASP A	291	-3.583	89.662 84.786	17.057	1.00	59.68
ATOM	2326	ō	ASP A	291	-3.867	84.552	16.743 17.828	1.00	33.13
ATOM	2327	N	SER A	292	-3.325	83.902	15.755	1.00 1.00	36.71 32.93
ATOM	2328	CA	SER A	292	-3.989	82.611	15.896	1.00	32.93
MOTA	2329	CB	SER A	292	-4.074	81.892	14.551	1.00	32.62
ATOM	2330	OG	SER A	292	-4.870	82.629	13.641	1.00	37.64
ATOM	2331	C .	SER A	292	-3.394	81.675	16.933	1.00	33.50
ATOM	2332	0	SER A	292	-2.223	81.310	16.870	1.00	35.88

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	2222	N	VAL A 2	93 -	4.223	81.283	17.889	1.00	35.69
ATOM	2333 2334				3.807	80.371	18.936	1.00	33.43
ATOM	2335				3.867	81.015	20.333	1.00	28.87
MOTA MOTA	2336			93 -	3.244	80.086	21.346	1.00	29.10
ATOM	2337			93 -	3.157	82.350	20.340	1.00	28.79 33.08
MOTA	2338		VAL A 2	93 -	4.754	79.193	18.925	1.00	33.08
ATOM	2339		VAL A 2	93 -	5.971	79.366	18.990	1.00	34.36
ATOM	2340	N			4.187	78.002	18.790 18.784	1.00	33.14
ATOM	2341	CA			4.952	76.770	17.458	1.00	33.14
ATOM	2342	CB			4.754	76.000 74.629	17.518	1.00	28.09
ATOM	2343	CG2	-		·5.426 ·5.318	76.832	16.303	1.00	29.00
MOTA	2344	CG1			-5.328	76.129	14.973	1.00	30.92
MOTA	2345	CD1			-4.476	75.952	19.983	1.00	36.82
ATOM	2346 2347	0			-3.277	75.882	20.273	1.00	40.13
ATOM ATOM	2348	N			-5.427	75.385	20.710	1.00	37.77
ATOM	2349	CA		295	-5.124	74.604	21.889	1.00	36.56 42.24
ATOM	2350	СВ	ASP A	295	-6.346	74.499	22.783	1.00	50.87
ATOM	2351	CG	ASP A		-6.163	75.234	24.071	1.00	60.02
ATOM	2352	OD1			-6.049	74.565	25.117 - 24.038	1.00	55.86
ATOM	2353	OD2	-		-6.092	76.481	21.544	1.00	35.69
ATOM	2354	С			-4.655	73.223 72.453	20.928	1.00	35.08
MOTA	2355	0			-5.384	72.433	21.955	1.00	35.13
MOTA	2356	N	-		-3.431 -2.488	73.736	22.692	1.00	34.11
ATOM	2357	CD	_		-2.466	71.563	21.690	1.00	35.32
ATOM	2358	CA			-1.478	71.653	22.368	1.00	33.77
ATOM	2359	CB CG		296	-1.169	73.116	22.339	1.00	35.72
ATOM	2360 2361	C		296	-3.689	70.463	22.327	1.00	38.35
ATOM	2362	0		296	-4.269	70.653	23.394	1.00	41.07
ATOM ATOM	2363	N	PHE A	297	-3.706	69.300	21.697	1.00	38.55 37.27
ATOM	2364	CA	PHE A	297	-4.455	68.180	22.208	1.00 1.00	34.45
ATOM	2365	CB	PHE A	297	-5.877	68.209	21.654 20.151	1.00	31.82
ATOM	2366	CG	PHE A	297	-5.957	68.187 67.025	19.475	1.00	30.97
ATOM	2367	CD1	PHE A	297	-6.324 -5.712	69.339	19.414	1.00	31.48
ATOM	2368	CD2	PHE A	297	-6.445	67.018	18.083	1.00	30.11
ATOM	2369	CE1	PHE A PHE A	297 297	-5.832	69.338	18.023	1.00	29.97
ATOM	2370	CE2 CZ	PHE A	297	-6.200	68.177	17.358	1.00	30.13
ATOM	2371	C	PHE A	297	-3.770	66.887	21.809	1.00	40.88
ATOM	2372 2373	0	PHE A	297	-2.954	66.865	20.891	1.00	43.86
ATOM ATOM	2374	N	ASP A	298	-4.064	65.806	22.511	1.00	44.53 48.48
ATOM	2375	CA	ASP A	298	-3.466	64.534	22.167	1.00 1.00	52.93
ATOM	2376	CB	ASP A	298	-2.590	64.015	23. 2 95 22.898	1.00	57.44
ATOM	2377	CG	ASP A	298	-1.808	62.778	21.778	1.00	54.35
MOTA	2378	OD1	ASP A	298	-2.020	62.254 62.333	23.705	1.00	66.50
MOTA	2379	OD2	ASP A	298 298	-0.964 -4.584	63.552	21.907	1.00	50.22
MOTA	2380	C	ASP A ASP A	298	-5.215	63.067	22.827	1.00	49.77
ATOM	2381	и	PRO A	299	-4.789	63.199	20.630	1.00	52.46
ATOM	2382 2383	CD	PRO A	299	-4.105	63.730	19.439	1.00	52.72
ATOM ATOM	2384	CA	PRO A	299	-5.835	62.266	20.230	1.00	56.64 54.35
ATOM	2385	CB	PRO A	299	-5.663	62.206	18.717	1.00 1.00	50.07
ATOM	2386	CG	PRO A	299	-5.165	63.564	18.388	1.00	63.86
MOTA	2387	С	PRO A	299	-5.648	60.898	20.868 20.687	1.00	69.53
ATOM	2388	0	PRO A	299	-6.492	60.011 60.712	21.580	1.00	68.69
ATOM	2389	N	MG A	300	-4.535 -4.231	59.449	22.250	1.00	73.13
MOTA	2390	CA	ARG A	300 300	-2.731	59.153	22.191	1.00	73.05
MOTA	2391	CB	ARG A ARG A	300	-2.732	58.825	20.810	1.00	75.18
MOTA	2392	CG CD	ARG A	300	-0.682	58.842	20.790	1.00	72.55
ATOM	2393	NE	ARG A	300	-0.165	60.144	21.181	1.00	71.35
MOTA	2394 2395	CZ	ARG A	300	0.867	60.748	20.595	1.00	71.94
ATOM ATOM	2396	NHI		300	1.506	60.171	19.579	1.00	73.46 71.10
ATOM	2397	NH2		300	1.274	61.934	21.032	1.00	76.43
ATOM	2398	С	arg A	300	-4.685	59.414	23.708	1.00 1.00	80.12
ATOM	2399	0	ARG A	300	-4.552	58.390	24.374 24.196	1.00	77.10
ATOM	2400	N	GLU A			60.536	24.196	1.00	81.37
ATOM	2401	CA	GLU A			_	26.331	1.00	82.38
ATOM	2402	CB	GLU A				26.422	1.00	89.06
MOTA	2403	CG	GLU A GLU A				27.750	1.00	94.30
MOTA	2404	_					28.115	1.00	97.83
MOTA	2405	OE:	א טעני						

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					2 241	61.201	28.425	1.00	97.36
ATOM	2406				-2.241	60.781	25.642	1.00	84.64
MOTA	2407			301	-7.193	61.498	24.836	1.00	83.56
ATOM	2408			301	-7.779		26.611	1.00	88.29
ATOM	2409	N	•	302	-7.849	60.122	27.527	1.00	89.03
ATOM	2410	CD :	PRO A	302	-7.263	59.114	26.800	1.00	87.98
MOTA	2411	CA	PRO A	302	-9.303	60.201	28.095	1.00	88.81
	2412		PRO A	302	-9.521	59.416		1.00	88.81
MOTA	2413		PRO A	302	-8.478	58.337	27.978	1.00	86.15
MOTA	2414			302	-9.804	61.652	26.925	1.00	85.57
MOTA				302	-10.737	62.060	26.236		84.86
MOTA	2415	_		303	-9.184	62.425	27.817	1.00	
MOTA	2416			303	-9.563	63.822	27.985	1.00	85.24
MOTA	2417			303	-8.929	64.404	29.254	1.00	89.02
ATOM	2418		ASN A	303	-9.217	65.900	29.433	1.00	93.08
ATOM	2419	CG		303	-8.501	66.589	30.150	1.00	95.61
MOTA	2420	OD1	ASN A		-10.242	66.401	28.755	1.00	95.94
ATOM	2421	ND2	ASN A			64.602	26.773	1.00	83.46
MOTA	2422	С	ASN A	303	-9.073	65.601	26.377	1.00	82.51
MOTA	2423	0	ASN A	303	-9.678	64.099	26.169	1.00	82.29
ATOM	2424	N	GLY A	304	-8.001		25.016	1.00	79.23
ATOM	2425	CA	GLY A	304	-7.413	64.745	25.513	1.00	77.89
ATOM	2426	С	GLY A	304	-6.639	65.945	24.802	1.00	78.97
	2427	0	GLY A	304	-6.503	66.945	26.748	1.00	76.87
MOTA	2428	N	LYS A	305	-6.156	65.855		1.00	76.76
ATOM		CA	LYS A	305	-5.403	66.938	27.348	1.00	78.46
MOTA	2429	СВ	LYS A	305	-5.585	66.962	28.880		82.23
MOTA	2430		LYS A	305	-4.408	66.440	29.691	1.00	
MOTA	2431	CG	LYS A	305	-3.751	67.539	30.519	1.00	85.07
ATOM	2432	CD		305	-2.573	66.997	31.311	1.00	88.93
MOTA	2433	CE	LYS A	305	-2.157	67.917	32.403	1.00	93.14
MOTA	2434	NZ	LYS A		-3.949	66.755	26.972	1.00	73.92
ATOM	2435	C	LYS A	305		65.623	26.867	1.00	73.27
ATOM	2436	0	LYS A	305	-3.474	67.855	26.797	1.00	72.39
ATOM	2437	N	SER A	306	-3.237	67.787	26.417	1.00	73.15
ATOM	2438	CA	SER A	306	-1.844		25.061	1.00	72.57
ATOM	2439	CB	SER A	306	-1.656	68.461	25.069	1.00	70.16
ATOM	2440	OG	SER A	306	-2.237	69.762	27.445	1.00	73.60
	2441	С	SER A	306	-0.982	68.474		1.00	71.26
MOTA	2442	Ö	SER A	306	-1.481	69.180	28.328	1.00	76.59
ATOM	2443	N	ASP A	307	0.314	68.208	27.363	1.00	78.33
MOTA		CA	ASP A	307	1.281	68.827	28.260		84.92
MOTA	2444	CB	ASP A	307	2.480	67.891	28.515	1.00	89.57
ATOM	2445	CG	ASP A	307		67.239	27.236	1.00	90.72
MOTA	2446		ASP A	307		67.902	26.515	1.00	
MOTA	2447	OD1	ASP A	307		66.065	26.956	1.00	90.72 74.93
MOTA	2448	OD2		307		70.130	27.593	1.00	
MOTA	2449	C	ASP A	307		71.163	28.254	1.00	73.18
ATOM	2450	0	ASP A			70.072	26.268	1.00	70.05
MOTA	2451	N	ARG A	308		71.212	25.471	1.00	64.62
ATOM	2452	CA	ARG A	308		70.877	23.986	1.00	64.91
MOTA	2453	CB	ARG A	308		69.738	23.570	1.00	65.23
MOTA	2454	CG	ARG A	308		69.720	22.067	1.00	65.31
MOTA	2455	CD	ARG A				21.573	1.00	68.52
MOTA	2456	NE	ARG A			68.494	21.800	1.00	69.44
MOTA	2457	CZ	ARG A	. 301		68.139	22.515	1.00	70.73
ATOM	2458	NH1	ARG A	30		68.925	21.334	1.00	71.60
	2459	NH2	ARG A	30		66.983		1.00	60.56
MOTA	2460	С	ARG A	30	8 1.422	72.394	25.695	1.00	62.91
MOTA	2461	ō	ARG A		8 0.211	72.243	25.786	1.00	58.75
MOTA		N	GLU F		9 2.016	73.576	25.721	1.00	59.53
MOTA	2462	CA	GLU A		9 1.278	74.807	25.937		64.51
MOTA	2463		GLU A			. 75 . 795	26.707	1.00	72.73
ATOM	2464	CB	GLU A			75.195	27.909	1.00	
MOTA	2465	CG				76.041	28.375	1.00	78.39
MOTA	2466	CD	GLU A			75.650	28.107	1.00	80.45
MOTA	2467	OE1				77.091	29.013	1.00	81.42
ATOM	2468						24.595	1.00	58.18
ATOM	2469	С	GLU		0.895		23.576	1.00	56.69
ATOM	2470	_	GLU		9 1.550		24.566	1.00	57.07
ATOM	2471		PRO		10 -0.202		25.662	1.00	58.98
MOTA	2472		PRO	A 3	10 -1.130			1.00	54.68
	2473			A 3	10 -0.639			1.00	56.45
ATOM	2474			A 3	10 -1.898			1.00	57.32
ATOM	2479				10 -1.67			1.00	49.05
ATOM		_	PRO		10 0.45		4	1.00	48.09
MOTA	2476	_	PRO		10 1.13				43.40
MOTA	247		LEU		11 0.61	7 77.835	21.512	1.00	43.40
MOTA	247	D 14	224	-					

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ATOM	2479	CA	LEU .	A 311	1.626	78.650	20.859		
ATOM	2480	CB	LEU .	A 311		77.726	20.839	1.00	36.12
ATOM ATOM	2481	CG	LEU A			78.324	19.578	1.00	32.22 31.79
ATOM	2482 2483	CD1				79.300	20.539	1.00	28.33
ATOM	2484	CD2 C				77.194	19.229	1.00	26.30
ATOM	2485	0	LEU A			79.478	19.793	1.00	32.51
ATOM	2486	N	SER A			78.915	18.903	1.00	35.00
ATOM	2487	CA	SER F		0.386	80.804	19.899	1.00	27.12
ATOM	2488	CB	SER A		0.324	81.654 83.123	18.894	1.00	26.22
ATOM	2489	OG	SER A		1.479	83.859	19.339 19.000	1.00	22.14
ATOM	2490	C	SER A	312	1.205	81.464	17.621	1.00 1.00	31.44
ATOM ATOM	2491	0	SER A		2.438	81.349	17.671	1.00	30.09 34.62
ATOM	2492 2493	N	TYR A		0.526	81.399	16.483	1.00	30.05
ATOM	2494	CA CB	TYR A		1.208	81.164	15.222	1.00	26.78
ATOM	2495	CG	TYR A		0.221	81.101	14.070	1.00	21.90
ATOM	2496	CD1	TYR A	-	0.740 0.464	80.223	12.968	1.00	23.94
ATOM	2497	CE1	TYR A		0.991	78.868 78.032	12.972	1.00	20.72
MOTA	2498	CD2	TYR A		1.555	80.729	12.022 11.951	1.00	22.06
ATOM	2499	CE2	TYR A		2.091	79.891	10.996	1.00	16.61
ATOM	2500	CZ	TYR A	313	1.792	78.541	11.041	1.00	16.69 17.14
ATOM ATOM	2501	ОН	TYR A	313	2.294	77.666	10.123	1.00	24.17
ATOM	2502 2503	C	TYR A	313	2.299	82.153	14.895	1.00	25.77
ATOM	2504	O N	TYR A	313	3.326	81.778	14.334	1.00	23.63
ATOM	2505	CA	GLY A GLY A	314 314	2.071	83.415	15.238	1.00	28.58
ATOM	2506	C	GLY A	314	3.053 4.370	84.444	14.965	1.00	34.94
ATOM	2507	0	GLY A	314	5.434	84.186 84.453	15.674	1.00	37.23
ATOM	2508	N	ASP A	315	4.301	83.683	15.117 16.906	1.00	41.94
ATOM	2509	CA	ASP A	315	5.498	83.388	17.682	1.00	37.16
ATOM	2510	CB	ASP A	315	5.162	83.140	19.157	1.00	33.44 37.41
ATOM ATOM	2511	CG	ASP A	315	4.707	84.406	19.881	1.00	40.95
ATOM	2512 2513	OD1 OD2	ASP A	315	3.906	84.295	20.835	1.00	48.93
ATOM	2514	C C	ASP A ASP A	315	5.147	85.515	19.504	1.00	45.51
ATOM	2515	0	ASP A	315 315	6.147 7.357	82.172	17.074	1.00	28.81
ATOM	2516	N	TYR A	316	5.333	82.139 81.179	16.893	1.00	32.18
ATOM	2517	CA	TYR A	316	5.823	79.963	16.746 16.116	1.00	26.31
ATOM	2518	CB	TYR A	316	4.646	79.064	15.709	1.00 1.00	25.28
ATOM	2519	CG	TYR A	316	4.986	77.997	14.682	1.00	23.80
ATOM ATOM	2520	CD1	TYR A	316	5.604	76.802	15.061	1.00	28.01 26.83
ATOM	2521 2522	CE1 CD2	TYR A	316	5.903	75.810	14.106	1.00	25.18
ATOM	2523	CE2	TYR A TYR A	316	4.682	78.177	13.323	1.00	22.23
ATOM	2524	CZ	TYR A	316 316	4.981 5.586	77.194	12.372	1.00	16.07
ATOM	2525	08	TYR A	316	5.850	76.020 75.040	12.769	1:00	19.33
ATOM	2526	С	TYR A	316	6.625	80.333	11.843 14.872	1.00	22.12
ATOM	2527	0	TYR A	316	7.812	80.010	14.766	1.00 1.00	26.20
ATOM	2528	N	LEU A	317	5.977	81.062	13.966	1.00	23.86 26.87
ATOM ATOM	2529	CA	LEU A	317	6.579	81.454	12.705	1.00	26.87
ATOM	2530 2531	CB CG	LEU A LEU A	317	5.548	82.112	11.783	1.00	22.99
ATOM	2532	CD1	LEU A	317	6.032	82.167	10.334	1.00	17.66
ATOM	2533	CD2	LEU A	317 317	5.962 5.205	80.780	9.722	1.00	16.43
ATOM	2534	c	LEU A	317	7.801	83.147 82.340	9.549	1.00	13.47
ATOM	2535	0	LEU A	317	8.781	82.125	12.830 12.134	1.00	25.42
MOTA	2536	N	GLN A	318	7.753	83.341	13.696	1.00 1.00	29.40
ATOM	2537	CA	GLN A	318	8.891	84.226	13.846	1.00	26.38 29.10
ATOM	2538	CB	GLN A	318	8.643	85.254	14.933	1.00	34.57
ATOM ATOM	2539 2540	CG	GLN A	318	7.722	86.361	14.557	1.00	45.89
ATOM	2541	CD OE1	GLN A	318	7.422	87.230	15.744	1.00	54.11
ATOM	2541	NE2	GLN A GLN A	318 318	8.276	87.996	16.198	1.00	60.92
ATOM	2543	C	GLN A		6.224 10.114	87.084	16.292	1.00	56.69
ATOM	2544	0	GLN A		11.147	83.429 83.529	14.215	1.00	32.19
ATOM	2545	N	ASN A	319	9.967	82.589	13.560 15.231	1.00	34.97
ATOM	2546	CA	ASN A		11.076	81.780	15.231	1.00	33.42
ATOM	2547	CB	ASN A		10.751	81.192	17.088	1.00	38.92 45.44
ATOM	2548	CG	ASN A		10.635	82.276	18.174	1.00	54.83
ATOM ATOM	2549	OD1	ASN A		11.612	82.952	18.502	1.00	56.44
ATOM	2550 2551	ND2 C	ASN A ASN A	319	9.429	82.470	18.702	1.00	59.48
·		_	A	319	11.506	80.705	14.725	1.00	40.03

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									1.00	44.50
		_	ASN A	319	12.703	80	.502	14.494	1.00	39.74
MOTA	2552	0	GLY A	320	10.531	80	.053	14.100	1.00	35.73
ATOM	2553	N	GLY A	320	10.827	79	.022	13.130	1.00	35.37
ATOM	2554	CA	GLY A	320	11. 61	1 79	.582	11 .962	1.00	37.50
MOTA	2555	С	GLY A	320	12.536	78	.951	11.471	1.00	34.76
ATOM	2556	0	LEU A	321	11 .27	0 80	.786	11. 530	1.00	39.63
ATOM	2557	N		321	11.967		.393	10.415	1.00	36.97
ATOM	2558	CA	LEU A	321	11.191	82	.583	9.877	1.00	38.18
MOTA	2559	CB	LEU A	321	9.901		.168	9.187	1.00	38.33
ATOM	2560	CG	LEU A	321	9.271		1.392	8.570	1.00	35.19
ATOM	2561	CD1	LEU A	321	10.181		1.108	8.134	1.00	44.08
ATOM	2562	CD2	LEU A		13.382		1.805	10.757		46.65
ATOM	2563	C	LEU A	321	14.28		1.606	9.953	1.00	49.49
MOTA	2564	0	LEU A	321	13.58		2.378	11.941	1.00	53.83
ATOM	2565	N	VAL A	322	14.92		2.806	12.345	1.00	53.89
ATOM	2566	CA	VAL A	322	14.93		3.617	13.671	1.00	53.18
ATOM	2567	CB	VAL A	322	13.94	5 8	4.767	13.615	1.00	55.17
ATOM	2568	CGl	VAL A	322	14.69	_	2.698	14.869	1.00	54.31
ATOM	2569	CG2	VAL A		15.89	٠ .	1.645	12.511	1.00	59.46
MOTA	2570	С	VAL A		17.10	_	1.848	12.478	1.00	52.61
MOTA	2571	0	A LAV		15.37		0.452	12.773	1.00	53.68
ATOM	2572	N	SER A		16.25	_	79.309	12.940	1.00	55.08
	2573	CA	SER A				78.096	13.468	1.00	
ATOM	2574	CB	SER F		15.48		77.644	12.551	1.00	52.98
ATOM	2575	OG	SER A		14.49		78.965	11.616	1.00	54.49
MOTA	2576	C	SER A				78.523	11.584	1.00	58.60
ATOM	2577	0	SER I				79.186	10.522	1.00	55.84
ATOM	2578	N	LEU				78.861	9.207	1.00	56.10
ATOM	2579	CA	LEU			23	78.485	8.229	1.00	52.73
MOTA	2580	CB	LEU				79.396	8.017	1.00	51.08
MOTA	2581	CG	LEU		_		80.431	6.945	1.00	54.72
MOTA	2582	CDI	LEU				78.561	7.606	1.00	50.43
ATOM	2583	CD		A 32			79.928	8.625	1.00	57.85
ATOM	2584	C	LEU	A 32			81.050	9.116	1.00	55.56
MOTA	2585	ō	LEU	A 32	4 17.6		79.536	7.595	1.00	62.83
MOTA	2586	N	ILE				80.428	6.910	1.00	64.52
MOTA		CA						5.969	1.00	64.56
MOTA	2587	CB					79.668	5.747	1.00	65.36
MOTA	2588	CG					80.496	6.516	1.00	65.53
ATOM	2589	CG				591	78.271	6.136	1.00	67.86
MOTA	2590	CE				563	77.197	6.034	1.00	65.56
ATOM	2591	C	ILE		25 18.	501	81.383	5.110	1.00	66.01
MOTA	2592	0	ILE			808	80.957	6.312	1.00	67.38
MOTA	2593		ASN		26 18.	.621	82.673	5.559	1.00	68.33
MOTA	2594	-				.899	83.696	6.105	1.00	73.56
MOTA	2595	_			26 18	.205	85.097	7.495	1.00	78.94
ATOM	2596	_				.632	85.325	8.171	1.00	83.34
ATOM	2597	_				.224	84.386	7.920	1.00	79.40
MOTA	2598					.590	86.582		1.00	65.53
MOTA	2599	_			26 18	.169	83.663	4.068 3.274	1.00	67.11
ATOM	2600	_				.254	83.861		1.00	59.01
ATOM	2603	_			327 19	.413	83.404	3.681	1.00	
MOTA	260		·	_		.761	83.355	2.263	1.00	
MOTA	260	· .		-		L.277	83.218	2.095	1.00	04
ATOM	260	-		_		2.021	84.515	2.327	1.00	60.90
MOTA	260	•				3.511	84.317	2.266	1.00	07
MOTA	260	•		. •		4.262	85.605	2.584	1.00	58.17
ATOM	260		~-	A SY	327 2	4.203	86.582		1.00	1
ATOM	260					9.033	82.256		- 0	0
MOTA	260	9	٠ .	YS A		8.610	82.472	0.370		
ATOM	263	70	٠.	YS A		8.868	81.088	2.109	- 0	
MOTA	26	11		SN A		8.186	79.980	1.439		1
MOTA	26			SN A		18.717	78.637	1.947		04
ATOM	26			SN A		20.104	78.349	5 1.410		4. 53
ATOM		14		SN A	_	21.052	79.05	6 1.729		
ATOM		15		ASN A	_	20.226	77.32	7 0.563		
MOTA		16		ASN A		16.657	80.01	3 1.49		
ATOM		17	_	ASN A		15.976	79.76	0 0.50		
		18		ASN A	•		80.29	1 2.68		
ATOM		519	• •	GLY A		16.117	80.34	0 2.86	4 1.	
ATOM	` .	620		GLY A		14.678	79.01	2 64	5 1.	
ATOM	•	621		GLY A		13.973	77.93		,5 1.	00 63.66
ATOM		622	0	GLY A	329	14.604			26 1.	00 63.44
ATON		623	N	GLN A	330	12.665		2 10		00 62.51
OTA	` _	624	CA	GLN A	330	11 .64	, , , , , , , ,	- -		
ATO	71 -									

					•	78 -			
ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM	2625 2626 2627 2628 2629 2630 2631 2632 2633 2634 2635 2637 2638 2639 2640 2641	CB CG CD OE1 NE2 C O CA CB OG1 CG2 C O OT MN MN	GLN A GLN A GLN A GLN A GLN A GLN A THR A	330 330 330 330 330 331 331 331 331 331		76.612 75.609 74.116 73.200 73.864 78.366 78.121 79.069 79.549 79.154 77.740 79.483 81.085 81.496 81.869 71.058 98.946	2.170 1.460 1.364 1.946 0.605 3.357 4.511 3.018 3.891 5.400 5.517 6.144 3.668 2.495 4.601 3.078 -5.069	1.00 1.00 1.00 1.00 1.00 1.00 1.00 1.00	61.84 62.53 61.91 56.42 56.02 61.76 61.83 57.39 46.65 38.61 48.69 59.73 55.52 62.34 32.10 40.69
END			MA A	351	16.765	98.946		1.00	32.10
EMD	-011	14154	MN A	351	16.765			1.00	32 10
	2641	MN	MN A	351	16 765		3.078	1.00	
	2641	MN	MN A	251			3.078	1 00	
ATOM	2641				10.357	71.058			62.34
ATOM	2640				8.131	81.869			
ATOM	2639	OT				81.496	2.495		
ATOM	2638	0				81.085	3.668		
	2637	C	THR A		-		6.144		·
		CG2	THR A				5.517	1.00	_
		OG1	THR A	331				1.00	
ATOM			THR A	331	9.685			1.00	57.39
ATOM				331	8.542				61.83
ATOM	2633				9.623	79.069			61.59
ATOM	2632	N				78.121	4.511		
	2631	0					3.357		
	2630	C	GLN A				0.605		
		NE2	GLN A	330			1.946	1.00	
			GLN A	330	•			1.00	
			GLN A	330	11.591			1.00	
ATOM				330	11.146			1.00	61.84
ATOM					12.152	76.612	2 170		
ATOM	2625	CB	CIN >						
					- 1	78 -			



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					- 79 -				
		0 71	500 10	1.000	<u>Table</u> 90.00 90	<u>د</u> 0.00 90.00			
CRYST1	46.80	0.0213		00000	0.000000		0.000000		
SCALE1 SCALE2		0.0000		13986	0.000000		0.000000		
SCALE3		0.0000		00000	0.009901		0.000000		7 03
ATOM	1	Cl	ACV	1	17.235	36.323	5.699	1.00	7.93 7.47
ATOM	2	C2	ACV	1	15.798	36.590	6.165 5.425	1.00	6.42
ATOM	3	C3	ACV	1	15.215	37.802	5.918	1.00	7.71
ATOM	4	C4	ACV	1	13.766 13.330	38.091 39.380	5.168	1.00	8.43
MOTA	5	C7	ACV	1 1	11.912	39.669	5.584	1.00	8.88
ATOM	6	C10 N11	ACV ACV	1	10.931	39.447	4.714	1.00	6.98
ATOM	7 8	C12	ACV	1	9.503	39.719	4.858	1.00	7.75
ATOM	9	C13	ACV	1	8.767	38.397	4.657	1.00	7.09
ATOM ATOM	10	N14	ACV	1	15.791	36.747	7.696	1.00	8.98
ATOM	11	015	ACV	1	11.566	40.061	6.715	1.00	11.68 7.15
ATOM	12	C16	ACV	1	9.131	40.743	3.765	1.00 1.00	8.44
MOTA	13	S17	ACV	1	9.513	40.068	2.102 4.670	1.00	9.78
MOTA	14	018	ACV	1	9.269	37.306 36.442	6.549	1.00	8.96
MOTA	15	019	ACV	1 1	18.173 17.393	36.068	4.492	1.00	7.91
MOTA	16	020 N29	ACV ACV	1	7.424	38.510	4.604	1.00	9.16
ATOM	17 18	C30	ACV	ì	6.543	37.341	4.409	1.00	9.68
ATOM ATOM	19	C31	ACV	1	5.317	37.433	5.318	1.00	10.48
ATOM	20	C32	ACV	1	6.104	37.147	2.912	1.00	12.78
ATOM	21	C33	ACV	1	7.348	36.829	2.039	1.00	11.31 18.82
ATOM	22	C37	ACV	1	5.562	38.560	2.564 6.210	1.00	10.58
MOTA	23	042	ACV	1	5.240	38.298	5.151	1.00	9.69
MOTA	24	043	ACV	1	4.417	36.560 14.100	2.417	1.00	25.69
ATOM	25	S	SUL	2 2	13.002 13.804	14.598	3.492	1.00	32.83
MOTA	26	01 02	SUL SUL	2	13.004	13.558	1.424	1.00	41.91
ATOM	27 28	03	SUL	2	12.155	13.073	2.934	1.00	30.42
MOTA MOTA	29	04	SUL	2	12.299	15.076	1.614	1.00	21.23
ATOM	30	FE	IUM	1000	7.903	40.943	0.544	1.00	7.64
ATOM	31	N	SER	3	-15.013	47.966	-1.402	1.00	42.72 39.06
ATOM	32	CA	SER	3	-14.317	46.679	-1.445	1.00	36.17
MOTA	33	С	SER	3	-12.942	46.953	-2.052 -2.493	1.00	41.73
ATOM	34	0	SER	3	-12.712	48.077 45.513	-2.197	1.00	42.74
ATOM	35	CB	SER SER	3 3	-14.951 -14.920	45.578	-3.613	1.00	52.50
MOTA	36	og n	VAL	4	-12.127	45.917	-2.096	1.00	33.45
ATOM	37 38	CA	VAL	4	-10.801	46.077	-2.708	1.00	30.02
ATOM ATOM	39	C	VAL	4	-10.826	45.243	-3.983	1.00	26.11
MOTA	40	0	VAL	4	-11.331	44.137	-3.995	1.00	26.45 32.20
ATOM	41	CB	VAL	4	-9.693	45.600	-1.751	1.00	31.47
ATOM	42	CG1	VAL	. 4	-8.324	45.544 46.380	-2.407 -0.434	1.00	39.65
MOTA	43	CG2	VAL	4	-9.619 -9.685	46.084	-7.342	1.00	28.73
ATOM	44	CB	SER SER	5 5	-10.494	46.429	-8.413	1.00	43.87
MOTA	45 46	OG C	SER	5	-9.128	43.958	-6.292	1.00	21.38
ATOM ATOM	47	0	SER	5	-8.126	44.094	~5.558	1.00	17.45
ATOM	48	N	SER	5	-10.297	45.742	-5.071	1.00	22.91 24.13
ATOM	49	CA	SER	5	-10.216	45.050	-6.347	1.00 1.00	20.27
ATOM	50	N	LYS	6	-9.338	42.900	-7.057 -7.199	1.00	18.92
ATOM	51	CA	LYS	6		41.770 40.516	-7.644	1.00	25.88
ATOM	52	CB	LYS	6 6		39.606	-8.620	1.00	33.15
ATOM	53	CG	LYS LYS	6		38.116	-8.377	1.00	36.92
ATOM	54 55	CD CE	LYS	6		37.434	-9.627	1.00	40.48
MOTA MOTA	56	NZ	LYS	6		38.278	-10.180	1.00	49.46
ATOM	57	C	LYS	6	-7.302	42.178	-8.167	1.00	16.57
ATOM	58	0	LYS	6		42.719	-9.294	1.00 1.00	19.33 13.66
ATOM	59	N	ALA	7		41.933	-7.756 -8.572	1.00	12.78
MOTA	60	CA	ALA	7		42.175	-7.716	1.00	14.08
MOTA	61	CB	ALA	7		42.083 41.135	-9.678	1.00	12.30
ATOM	62	C	ALA		7 -4.803 7 -5.069	39.957	-9.497	1.00	13.11
ATOM	63	0	ALA ASN		7 -5.069 3 -4.325	41.585	-10.844	1.00	15.13
ATOM	64	N CA	ASN		3 -4.026	40.653	-11.913	1.00	16.54
ATOM	65 66	CB	ASN		3 -3.650	41.448	-13.197	1.00	24.27
MOTA MOTA	67	CG	ASN		8 -4.274	40.597	-14.298	1.00	29.61
ATOM	68	OD1			8 -3.669	39.640	-14.787	1.00	35.60 43.75
ATOM	69	ND2	ASN		8 -5.528	40.986	-14.477	1.00	33.13

						00			
ATOM	70	С	ASN	8	-2.738	39.882	-11.623	1.00	13.63
ATOM	71	0	ASN	8		40.451	-11.691	1.00	16.79
ATOM ATOM	72	N	VAL	9		38.611	-11.303	1.00	11.43
ATOM	73 74	CA	VAL	9		37.707	-11.016	1.00	10.00
ATOM	74 75	CB	VAL	9		37.383	-9.522	1.00	10.55
ATOM	75 76	CG1		9		36.537	-9.229	1.00	10.77
ATOM	76 77	CG2 C		9	-1.726	38.675	-8.725	1.00	11.32
ATOM	7.7 7.8	0	VAL VAL	9	-1.955	36.422	-11.845	1.00	10.66
ATOM	79	N	PRO	9	-2.621	35.466	-11.464	1.00	14.19
ATOM	80	CD	PRO	10 10	-1.385	36.425	-13.059	1.00	9.44
ATOM	81	CA	PRO	10	-0.544 -1.565	37.474	-13.650	1.00	10.90
ATOM	82	СВ	PRO	10	-0.901	35.299 35.749	-13.942	1.00	10.48
ATOM	83	CG	PRO	10	-0.067	36.924	-15.235	1.00	12.92
ATOM	84	С	PRO	10	-0.883	34.026	-14.937	1.00	15.89
ATOM	85	0	PRO	10	0.125	34.020	-13.444 -12.734	1.00	9.89
ATOM	86	N	LYS	11	-1.414	32.896	-13.847	1.00	10.22
ATOM	87	CA	LYS	11	-0.815	31.597	-13.586	1.00	9.52
ATOM	88	CB	LYS	11	-1.885	30.560	-13.230	1.00	9.53
ATOM	89	CG	LYS	11	-2.651	30.971	-11.965	1.00	12.58
ATOM	90	CD	LYS	11	-3.746	30.048	-11.504	1.00	18.45 23.78
ATOM	91	CE	LYS	11	-4.685	30.872	-10.629	1.00	25.46
ATOM	92	NZ	LYS	11	-4.154	31.101	-9.250	1.00	27.77
ATOM	93	С	LYS	11	0.020	31.211	-14.803	1.00	10.29
ATOM	94	0	LYS	11	-0.482	31.172	-15.926	1.00	16.95
ATOM	95	N	ILE	12	1.301	31.019	-14.640	1.00	8.18
ATOM	96	CA	ILE	12	2.214	30.697	-15.742	1.00	8.29
ATOM	97	CB	ILE	12	3.358	31.733	-15.815	1.00	8.64
ATOM ATOM	98	CG2	ILE	12	4.366	31.311	-16.864	1.00	9.33
ATOM	99	CG1	ILE	12	2.860	33.160	-16.018	1.00	9.90
ATOM	100 101	CD1	ILE	12	3.945	34.238	-15.984	1.00	10.28
ATOM	101	С 0	ILE	12	2.749	29.284	-15.518	1.00	7.89
ATOM	102	N	ILE	12	3.346	28.974	-14.504	1.00	7.80
ATOM	104	CA	ASP ASP	13	2.542	28.428	-16.522	1.00	8.72
ATOM	105	CB	ASP	13 13	3.109	27.068	-16.533	1.00	8.16
ATOM	106	CG	ASP	13	2.391	26.193	-17.536	1.00	9.68
ATOM	107	OD1	ASP	13	2.947 4.047	24.828	-17.728	1.00	11.65
ATOM	108	OD2	ASP	13	2.283	24.478 24.013	-17.257	1.00	10.88
ATOM	109	С	ASP	13	4.601	27.248	-18.401 -16.838	1.00	19.22
MOTA	110	0	ASP	13	5.005	27.527	-17.990	1.00	7.72
ATOM	111	N	VAL	14	5.413	26.983	-15.825	1.00	9.02
ATOM	112	CA	VAL	14	6.862	27.170	-15.947	1.00	8.27
ATOM	113	CB	VAL	14	7.453	27.766	-14.680	1.00	8.27
ATOM	114	CG1	VAL	14	6.890	29.164	-14.465	1.00	8.09 9.81
ATOM	115	CG2	VAL	14	7.298	26.882	-13.458	1.00	8.58
ATOM	116	С	VAL	14	7.592	25.910	-16.328	1.00	8.98
ATOM	117	0	VAL	14	8.815	25.950	-16.464	1.00	10.04
ATOM	118	N	SER	15	6.851	24.822	-16.531	1.00	9.65
ATOM ATOM	119	CA	SER	15	7.532	23.572	-16.883	1.00	9.94
ATOM	120	CB	SER	15	6.548	22.411	-16.994	1.00	10.80
ATOM	121	OG	SER	15	5.618	22.532	-18.063	1.00	12.34
ATOM	122 123	C	SER	15	8.469	23.599	-18.070	1.00	9.33
ATOM	124	N O	SER	15	9.519	22.915	-18.009	1.00	9.96
ATOM	125	CD	PRO PRO	16 16	8.218	24.364	-19.141	1.00	10.18
ATOM	126	CA	PRO	16	7.026	25.108	-19.546	1.00	9.79
ATOM	127	CB	PRO	16	9.220	24.381	-20.209	1.00	10.12
ATOM	128	CG	PRO	16	8.629 7.127	25.357	-21.226	1.00	10.60
ATOM	129	c	PRO	16	10.583	25.247	-21.015	1.00	11.12
ATOM	130	ō	PRO	16	11.579	24.909 24.613	-19.807	1.00	9.66
ATOM	131	N	LEU	17	10.666		-20.444	1.00	11.72
ATOM	132	CA	LEU	17	11.949	25.693 26.232	-18.711	1.00	10.05
ATOM	133	CB	LEU	17	11.738		-18.288	1.00	10.06
ATOM	134	CG	LEU	17	10.992	27.358 28.598	-17.276	1.00	8.52
ATOM	135	CD1	LEU	17	10.784	29.540	-17.808 -16.622	1.00	9.04
ATOM	136	CD2	LEU	17	11.738	29.340	-18.622	1.00	9.12
ATOM	137	C	LEU	17	12.890	25.183	-18.922	1.00	10.89
ATOM	138	0	LEU	17	14.087	25.442	-17.466	1.00	11.62
ATOM	139	N	PHE	18	12.403	23.970	-17.499	1.00	12.52
ATOM	140	CA	PHE	18	13.234	22.862	-17.065	1.00	11.77
ATOM	141	CB	PHE	18	12.363	21.947	-16.180	1.00	12.92
MOTA	142	CG	PHE	18	12.070	22.571	-14.820	1.00	12.94
								1.00	13.53

110 75.23						81 -				
								-14.598	1.00	17.84
	1.4.7	CD1	PHE		10.872			-13.766	1.00	14.00
ATOM	143 144	CD2	PHE		12.965		.503	-13.359	1.00	17.86
ATOM	145	CEl	PHE		10.537		.720	-12.519	1.00	14.38
ATOM	146	CE2	PHE	19	12.638		.974	-12.326	1.00	15.20
ATOM	147	CZ	PHE	18	11.444		.614	-18.231	1.00	14.72
MOTA	148	C	PHE	18	13.768		.054	-18.012	1.00	17.55
ATOM		0	PHE	18	14.567		.129	-19.445	1.00	15.60
ATOM	149	И	GLY	19	13.321		349	-20.583	1.00	17.05
MOTA	150	CA	GLY	19	13.718		513	-21.663	1.00	16.88
ATOM	151	C	GLY	19	14.489		2.248	-21.384	1.00	16.84
MOTA	152	0	GLY	19	15.092		3.280	-22.868	1.00	18.23
ATOM	153	N	ASP	20	14.471		1.679	-23.997	1.00	19.57
ATOM	154	CA	ASP	20	15.241		2.147	-25.186	1.00	16.96
ATOM	155	C	ASP	20	14.418	3 2	2.595	-26.285	1.00	18.78
MOTA	156	0	ASP	20	14.976		2.646	-24.491	1.00	25.96
ATOM	157	СВ	ASP	20	16.17		1.025	-23.320	1.00	30.78
ATOM	158	CG	ASP	20	16.95	-	0.446	-23.320	1.00	38.92
MOTA	159	OD1	ASP	20	17.10	_	9.208		1.00	40.12
ATOM	160	OD2	ASP	20	17.31	-	1.213	-22.393 -25.013	1.00	16.58
MOTA	161		ASP	21	13.16	1 2	2.913		1.00	16.91
ATOM	162	N	ASP	21	12.38	-	13.435	-26.145	1.00	18.23
MOTA	163	CA	ASP	21	10.92	.0 2	23.028	-25.985	1.00	20.86
ATOM	164	CB	ASP	21	10.02		23.362	-27.142	1.00	21.70
MOTA	165	CG	ASP	21	10.31		24.380	-27.796	1.00	27.79
MOTA	166	OD1	ASP	21	8.96	58	22.756	-27.430	1.00	14.20
ATOM	167	OD2		21	12.56		24.961	-26.116	1.00	12.84
ATOM	168	C	ASP	21	11.89		25.648	-25.343	1.00	15.68
MOTA	169	0	ASP	22	13.50		25.500	-26.887	1.00	13.82
MOTA	170	N	GLN	22	13.8		26.915	-26.764		13.58
MOTA	171	CA	GLN	22			27.347	-27.545	1.00 1.00	15.37
MOTA	172	CB	GLN	22			26.474	-27,348		16.56
ATOM	173	CG	GLN		_		26.189	-25.918	1.00	19.01
ATOM	174	CD	GLN	22			27.042	-25.067	1.00	19.39
ATOM	175	OE1	GLN	22			24.984	-25.728	1.00	13.52
ATOM	176	NE2	GLN	22			27.819	-27.116	1.00	11.96
ATOM	177	С	GLN	2.2			28.853	-26.449	1.00	
ATOM	178	0	GLN	22	_		27.480	-28.125	1.00	16.53
ATOM	179	N	ALA	23			28.320	-28.488	1.00	16.41
ATOM	180	CA	ALA	2.			27.855	-29.796	1.00	22.56
	181	CB	ALA	2.			28.331	-27.352	1.00	13.99
ATOM	182	C	ALA	2	-	715	29.380	-27.065	1.00	13.68
ATOM	183	0	ALA	2		120	27.160	-26.761	1.00	13.08
MOTA MOTA	184	N	ALA	2		451	27.122	-25.650	1.00	11.55
MOTA	185	CA	ALA	2		481	25.694	-25.217	1.00	13.62
	186	CB	ALA		_	214	27.977	-24.524	1.00	9.62
MOTA ATOM	187	С	ALA			988	28.627	-23.815	1.00	9.80
ATOM	188	0	ALA			213	27.958	-24.263	1.00	10.01
	189	N	LYS			. 278	28.781	-23.178	1.00	9.16
ATOM	190	CA	LYS			. 844	28.472	-23.004	1.00	9.87
ATOM	191					.332	27.128	-22.327	1.00	13.94
ATOM	192		LYS			.600	27.106	-21.852	1.00	21.25
ATOM	193					.077	25.974	-22.406	1.00	24.07
ATOM	194					.817	26.073	-22.150	1.00	19.05
ATOM	195		Z LYS			. 254	30.249	-23.474	1.00	7.92
MOTA	196	_	LYS			.657	31.042	-22.566	1.00	8.19
MOTA	197	_	LYS			1.375		-24.728	1.00	8.75
ATOM	198					.811	30.662		1.00	9.12
MOTA	199	-				.564	32.085		1.00	9.73
MOTA	200	_	B MET			0.903	32.408		1.00	10.03
MOTA	20	-	G MET			2.399	32.424	050	1.00	10.21
MOTA	20		D MET			3.322	33.724		1.00	10.95
MOTA			E MET			3.056	35.132		1.00	
MOTA	20	-	MET		26	9. 1 15	32.487		1.00	
MOTA	20	· .	MET		_	8.828	33.594		1.00	- 40
MOTA	20		N ARG			8.163	31.585	04 000	1.00	
MOTA	20		CA ARC		27	6.767	31.90			
MOTA	20	•	CB ARC		27	5.842	30.89			
MOTA	20		CG ARG		27	5.895	31.04			
MOTA		• •			27	4.969	30.14			
MOTA					27	5.322	28.73			·
MOTA					27	5.998	28.01			
ATOM		12			27	6.271	26.72	20 (2)		
ATOM		13			27	6.357	28.59		=	
MOTA		14	• • • • • • • • • • • • • • • • • • • •		27	6.496	32.02	-23.319	, 1.0	
MOTA	2	15	C AR							

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ATOM	:	216	О А	RG	27 #				
ATOM		217		AL			854 -22.92	25 1 0	0
MOTA	2	218		AL		214 31.	249 -22.48		
MOTA		219				129 31.	447 -21.03		
ATOM		20		AT.	28 7.	799 30.	307 -20.27		
ATOM				AT.	28 7.	803 30.			8.02
ATOM		21	CG2 V	L		184 28.9		2 1.00	9.37
ATOM		22	C V	T.					10.98
		23	O VA	L				3 1.00	-0.50
ATOM	2	24	N AL					3 1.00	
ATOM	2	25	CA AL			93.0	096 -21.23	5 1.00	,.,0
ATOM	2:	26	CB AL		29 9.5		368 -20.94		7.04
ATOM			_	_	29 10.8	70 34.4	47 -21.74		,.,,
ATOM			_		29 8.6	91 35.5			
ATOM	22				29 8.6	62 36.5			
ATOM			N GLI	1	30 7.9	02 35.4	^ ~	1.00	8.13
ATOM	23		CA GLI	1	30 7.0				7.11
	23		CB GL1	1	30 6.2				7.56
ATOM	23	2 (CG GLM	_				1.00	
ATOM	23	3 (CD GLA					1.00	8.19
ATOM	23		E1 GLN				35 -23 845	00	8.58
ATOM	23				3.39		-23.534		8.95
ATOM	23	-		_	0 3.57	70 38.74			10.78
ATOM		-		_	0 6.00		-5.101	1.00	9.99
ATOM	23	_		3	0 5.63			1.00	6.94
ATOM	238		GLN	3	1 5.46			1.00	8.27
	239		A GLN	3		,		1.00	7.41
ATOM	240) C		3		,2		1.00	
ATOM	241	C					7 -19.675	1.00	7.30
ATOM	242			3			8 -20.829		8.13
ATOM	243			3 :		2 32.31	6 -20.493	1.00	9.37
ATOM	244			3 :	1.84	32.090	0 -19.656	1.00	11.83
ATOM			E2 GLN	3 1	L 3.39:	31.36		1.00	15.21
ATOM	245	_	GLN	3 1	5.093		~ 0 0	1.00	18.42
ATOM	246	-	GLN	3 1		576		1.00	7.43
	247	N	ILE	32			-0.027	1.00	7.98
ATOM	248	CA	ILE	32			-0.50/	1.00	6.96
ATOM	249	CB		32				1.00	
ATOM	250	CG					-17.010	1.00	7.29
ATOM	251	CG		32		36.685	-16.004		7.37
ATOM	252	CD		32		34.504	-16.497	1.00	9.11
ATOM	253			32	9.335	33.611		1.00	7.84
ATOM		C	ILE	32	7.235	38.139		1.00	9.10
ATOM	254	0	ILE	32	7.023			1.00	7.13
	255	N	ASP	33	7.632	38.945	-0.002	1.00	8.31
ATOM	256	CA	ASP	33		38.515	-18.717	1.00	
ATOM	257	CB	ASP	33	7.801	39.927	-19.072	1.00	7.76
ATOM	258	CG	ASP		8.257	40.026	-20.550	1.00	8.04
ATOM	259	OD1		33	8.447	41.482	-20.994		8.19
ATOM	260	OD2	-	33	9.429	42.118	-20.550	1.00	8.88
ATOM	261			33	7.560	41.941	-21.792	1.00	9.63
ATOM		C	ASP	33	6.480	40.675		1.00	9.07
ATOM	262	0	ASP	33	6.480	41.751	-18.835	1.00	7.95
	263	N	ALA	34	5.357		-18.200	1.00	8.54
ATOM	264	CA	ALA	34		40.154	-19.355	1.00	
ATOM	265	CB	ALA	34	4.079	40.834	-19.202	1.00	8.10
ATOM	266	С	ALA	34	2.993	40.062	-19.938	1.00	8.69
ATOM	267	0	ALA		3.709	41.028	-17.735		9.24
ATOM	268	N		34	3.284	42.105	-17.299	1.00	8.36
ATOM	269		ALA	35	3.903	39.967	-16.933	1.00	9.82
ATOM	270	CA	ALA	35	3.505	40.093		1.00	8.64
ATOM		CB	ALA	35	3.527	38.723	-15.538	1.00	9.10
ATOM	271	С	ALA	35	4.423	41.047	-14.870	1.00	11.05
	272	0	ALA	35	3.968	41.04/	-14.779	1.00	9.17
ATOM	273	N	SER	36	5.709	41.822	-13.942	1.00	10.62
ATOM	274	CA	SER	36		41.042	-15.146	1.00	
MOTA	275	CB	SER		6.683	41.896	-14.467	1.00	8.20
ATOM	276	OG	SER	36	8.108	41.485	-14.830		7.99
ATOM	277	C		36	8.354	40.129	-14.485	1.00	8.90
ATOM	278		SER	36	6.436	43.364	-14.801	1.00	8.75
ATOM		0	SER	36	6.761	44.224	13.001	1.00	9.43
ATOM	279	N	ARG	37	5.871	43.633	-13.994	1.00	12.45
ATOM	280	CA	ARG	37	5.572	44.996	-15.993	1.00	9.00
	281	CB	ARG	37	5.685	11.996 45.00°	-16.415	1.00	10.53
ATOM	282	CG	ARG	37		45.095	-17.931	1.00	
ATOM	283	CD	ARG		7.046	44.858	-18.544	1.00	11.22
ATOM	284	NE	ARG	37	7.074	44.615	-20.051		12.00
ATOM	285	CZ		37	6.514	45.706	-20.881	1.00	14.37
ATOM	286		ARG	37	6.327	45.575	-22.190	1.00	15.54
ATOM		NH1	ARG	37	6.682	44.430	-27 70-	1.00	15.00
ATOM	287	NH2	ARG	37	5.812	46.595	-22.781	1.00	16.31
011	288	C	ARG	37	4.204		-22.875	1.00	14.87
						45.459	-15.925		11.82
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ATOM	289	0	ARG	37	3.914	46.654	-15.947	1.00	17.60
ATOM	290	N	ASP	38	3.367	44.520	~15.475	1.00	12.19
ATOM	291	CA	ASP	38	2.045	44.889	-14.976	1.00	14.66
ATOM	292	CB	ASP						
				38	1.017	43.860	-15.463	1.00	16.65
MOTA	293	CG	ASP	38	-0.441	44.105	-15.173	1.00	17.06
ATOM	294	OD1	ASP	38	-0.763	45.278	-14.922	1.00	22.39
ATOM	295	OD2	ASP	38	-1.316	43.219	-15.263	1.00	20.09
MOTA	296	С	ASP	38	2.102	45.018	-13.455	1.00	13.71
ATOM	297	ō	ASP	38	2.736	45.927	-12.904	1.00	
									14.27
ATOM	298	N	THR	39	1.460	44.073	-12.737	1.00	11.56
ATOM	299	CA	THR	39	1.415	44.205	-11.298	1.00	11.81
ATOM	300	CB	THR	39	0.320	43.390	-10.584	1.00	14.06
ATOM	301	OG1	THR	39	0.687	41.990	-10.698	1.00	17.03
MOTA	302	CG2	THR	39	-1.008	43.691	-11.223	1.00	17.60
ATOM	303	С	THR	39	2.721	43.776	-10.634	1.00	10.17
ATOM	304	ō	THR	39	2.920				
						44.118	-9.459	1.00	11.25
ATOM	305	N	GLY	40	3.510	42.982	-11.367	1.00	9.14
ATOM	306	CA	GLY	40	4.740	42.526	-10.777	1.00	8.52
ATOM	307	C	GLY	40	4.618	41.178	-10.115	1.00	9.63
ATOM	308	0	GLY	40	5.587	40.753	-9.505	1.00	14.89
ATOM	309	N	PHE	41	3.477	40.522	-10.124	1.00	8.18
ATOM	310	CA	PHE	41	3.307	39.207	-9.532		
ATOM			PHE	41				1.00	7.48
	311	CB			2.353	39.290	-8.343	1.00	7.50
ATOM	312	CG	PHE	41	2.952	39.927	-7.078	1.00	7.93
ATOM	313	CD1	PHE	41	2.936	41.286	-6.859	1.00	8.43
ATOM	314	CD2	PHE	41	3.499	39.110	-6.100	1.00	7.47
ATOM	315	CE1	PHE	41	3.446	41.812	-5.683	1.00	8.79
ATOM	316	CE2	PHE	41	4.040	39.635	-4.933	1.00	
ATOM		CZ							8.21
	317		PHE	41	4.032	40.998	-4.757	1.00	8.46
MOTA	318	С	PHE	41	2.782	38.226	-10.550	1.00	6.88
ATOM	319	0	PHE	41	1.952	3 8.554	-11.401	1.00	9.03
ATOM	320	N	PHE	42	3.164	36.978	-10.374	1.00	6.68
ATOM	321	CA	PHE	42	2.539	35.845	-11.075	1.00	6.92
ATOM	322	CB	PHE	42	3.148	35.586	-12.456	1.00	7.96
ATOM	323	CG	PHE	42					
					4.564	35.072	-12.516	1.00	7.35
MOTA	324	CD1	PHE	42	4.802	33.699	-12.586	1.00	7.79
ATOM	325	CD2	PHE	42	5.637	35.931	-12.518	1.00	8.85
ATOM	326	CE1	PHE	42	6.124	33.266	-12.696	1.00	8.64
ATOM	327	CE2	PHE	42	6.951	35.498	-12.656	1.00	9.37
ATOM	328	CZ	PHE	42	7.193	34.141	-12.740	1.00	9.28
ATOM	329	C	PHE	42	2.620	34.594	-10.216	1.00	6.60
ATOM	330	0	PHE	42	3.489	34.518	-9.338		
								1.00	6.98
ATOM	331	N	TYR	43	1.783	33.606	-10.477	1.00	6.57
ATOM	332	CA	TYR	43	1.913	32.290	-9.860	1.00	6.96
ATOM	333	CB	TYR	43	0.575	31.694	-9.466	1.00	7.72
ATOM	334	CG	TYR	43	0.098	32.111	-8.088	1.00	7.41
MOTA	335	CD1	TYR	43	-0.901	33.078	-7.938	1.00	8.92
ATOM	336	CE1	TYR	43	-1.335	33.480	-6.697	1.00	9.19
ATOM	337	CD2	TYR	4.3	0.664	31.618	-6.939	1.00	7.76
ATOM	338	CE2	TYR	43	0.248	32.035	-5.690	1.00	8.82
ATOM	339	CZ	TYR	43	-0.715	32.992	-5.574	1.00	9.99
ATOM	340	OH	TYR	43	-1.130	33.349	-4.303	1.00	11.00
MOTA	341	C	TYR	43	2.625	31.390	-10.867	1.00	6.77
ATOM	342	0	TYR	43	2.160	31.203	-11.985	1.00	9.17
ATOM	343	N	ALA	44	3.663	30.736	-10.386	1.00	6.74
ATOM									
	344	CA	ALA	44	4.321	29.654	-11.138	1.00	6.80
ATOM	345	CB	ALA	44	5.766	29.522	-10.683	1.00	6.89
MOTA	346	C	ALA	44	3.590	28.345	-10.834	1.00	6.81
ATOM	347	0	ALA	44	3.423	27.965	-9.679	1.00	7.69
ATOM	348	N	VAL	45	3.075	27.695	-11.849	1.00	7.45
ATOM	349	CA	VAL	45	2.373	26.431	-11.766	1.00	7.41
ATOM	350	CB	VAL	45	0.902	26.570	-12.161	1.00	9.68
ATOM			VAL						
	351	CG1		45	0.228	27.601	-11.255	1.00	10.94
ATOM	352	CG2	VAL	45	0.670	26.895	-13.632	1.00	10.29
ATOM	353	C	VAL	45	3.120	25.384	-12.583	1.00	7.22
MOTA	354	0	VAL	45	3.984	25.718	-13.393	1.00	7.51
ATOM	355	N	ASN	46	2.862	24.095	-12.325	1.00	8.30
ATOM	356	CA	ASN	46	3.565	22.985	-12.948	1.00	8.32
ATOM	357	CB	ASN	46	3.323	22.885	-14.449	1.00	11.81
ATOM		CG	ASN	46			-14.786		
	358				1.875	22.704		1.00	18.20
ATOM	359	OD1	ASN	46	1.395	21.610	-14.470	1.00	31.96
ATOM	360	ND2	ASN	46	1.269	23.750	-15.306	1.00	24.56
MOTA	361	C	ASN	46	5.043	23.111	-12.634	1.00	8.17

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MOTA	362	0	ASN	46	5.936	22.860	-13.449	1.00	10.28
ATOM	363	N	HIS	47	5.323	23.425	-11.366	1.00	8.42
MOTA	364	CA	HIS	47	6.663	23.646	-10.843	1.00	8.14
ATOM	365	CB	HIS	47	6.618	24.724	-9.775	1.00	8.35
ATOM	366	CG	HIS	47	5.590	24.430	-8.727 -8.504	1.00	7.34
ATOM	367	CD2	HIS	47	4.399	25.000	-8.304	1.00	7.88 7.39
ATOM	368 369	ND1 CE1	HIS HIS	47 47	5.7 1 9 4.626	23.383 23.360	-7.052	1.00	8.04
ATOM ATOM	370	NE2	HIS	47	3.827	24.344	-7.440	1.00	8.14
ATOM	371	C	HIS	47	7.375	22.430	-10.325	1.00	7.89
ATOM	372	0	HIS	47	8.580	22.464	-10.091	1.00	9.85
ATOM	373	N	GLY	48	6.691	21.328	-10.139	1.00	8.33
ATOM	374	CA	GLY	48	7.238	20.053	-9.749	1.00	8.83
MOTA	375	С	GLY	48	7.522	19.849	-8.282	1.00	8.46
ATOM	376	0	GLY	48	8.060	18.780	-7.953	1.00	11.24
MOTA	377	N	ILE	49	7.267	20.817	-7.412	1.00	7.06
ATOM	378	CA	ILE	49	7.568	20.636	-6.015 -5.389	1.00 1.00	6.70 7.04
ATOM	379	CB	ILE	49 49	8.093 8.286	21.962 21.829	-3.886	1.00	7.67
MOTA MOTA	380 381	CG2 CG1	ILE	49	9.383	22.383	-6.077	1.00	8.13
ATOM	382	CD1	ILE	49	9.964	23.699	-5.584	1.00	9.61
ATOM	383	C	ILE	49	6.327	20.166	-5.245	1.00	6.55
ATOM	384	0	ILE	49	5.210	20.605	-5.497	1.00	7.34
ATOM	385	N	ASN	50	6.531	19.246	-4.311	1.00	6.14
ATOM	386	CA	ASN	50	5.449	18.729	-3.464	1.00	5.89
ATOM	387	CB	ASN	50	5.834	17.332	-2.967	1.00	6.25
ATOM	388	CG	ASN	50	4.688	16.658	-2.270	1.00	5.80
ATOM	389	OD1	ASN	50	3.717	17.297	-1.870	1.00	7.60
ATOM	390	ND2	ASN	50	4.840	15.366	-2.058	1.00 1.00	7.26 5.68
ATOM	391	C	asn asn	50 50	5.184 5.744	19.714 19.597	-2.331 -1.230	1.00	6.62
ATOM	392 393	N	VAL	51	4.328	20.676	-2.619	1.00	5.97
ATOM ATOM	394	CA	VAL	51	4.037	21.706	-1.632	1.00	6.10
MOTA	395	CB	VAL	51	3.508	23.010	-2.290	1.00	6.74
ATOM	396	CG1	VAL	51	4.557	23.676	-3.184	1.00	9.06
ATOM	397	CG2	VAL	51	2.250	22.743	-3.048	1.00	9.15
ATOM	398	C	VAL	51	3.137	21.232	-0.504	1.00	7.22
ATOM	399	0	VAL	51	3.199	21.758	0.610	1.00	7.84
ATOM	400	N	GLN	52	2.286	20.231	-0.761	1.00	7.44
ATOM	401	CA	GLN	52	1.474	19.721	0.339	1.00	6.88 8.70
ATOM	402	CB	GLN	52 53	0.442 -0.534	18.728 18.205	-0.163 0.917	1.00 1.00	10.71
ATOM ATOM	403 404	CG CD	GLN GLN	52 52	-0.334	17.059	1.807	1.00	12.39
MOTA	405	OE1	GLN	52	0.970	16.387	1.579	1.00	12.25
ATOM	406	NE2	GLN	52	-0.672	16.925	2.956	1.00	13.45
ATOM	407	C	GLN	52	2.410	19.094	1.378	1.00	6.81
ATOM	408	0	GLN	52	2.162	19.264	2.599	1.00	6.97
ATOM	409	N	ARG	53	3.434	18.364	0.950	1.00	6.70
ATOM	410	CA	ARG	53	4.339	17.734	1.912	1.00	6.00
MOTA	411	CB	ARG	53	5.152	16.655	1.210	1.00	6.55
ATOM	412	CG	ARG	53	6.068	15.894	2.129	1.00	6.59
ATOM	413	CD	ARG	53	6.645	14.676	1.432 2.348	1.00 1.00	8.72 8.70
ATOM	414	NE	ARG ARG	53 53	7.445 8.771	13.846 13.910	2.425	1.00	10.05
ATOM ATOM	415 416	CZ NH1	ARG	53	9.464	14.723	1.605	1.00	12.80
ATOM	417	NH2	ARG	53	9.424	13.106	3.279	1.00	10.00
ATOM	418	С	ARG	53	5.156	18.809	2.598	1.00	5.84
ATOM	419	ō	ARG	53	5.396	18.698	3.820	1.00	6.89
MOTA	420	N	LEU	54	5.598	19.850	1.903	1.00	5.98
ATOM	421	CA	LEU	54	6.274	20.982	2.544	1.00	5.87
ATOM	422	CB	LEU	54	6.558	22.056	1.489	1.00	6.27
MOTA	423	CG	LEU	54	6.940	23.435	2.017	1.00	7.00
ATOM	424	CD1	LEU	54	8.286	23.396	2.689	1.00	7.98
ATOM	425	CD2	LEU	54 54	6.864	24.441	0.866	1.00 1.00	8.66 5.97
MOTA	426	C	LEU	54 54	5.406 5.870	21.576 21.822	3.660 4.788	1.00	6.89
ATOM	427 428	O N	LEU SER	55	4.136	21.786	3.344	1.00	6.27
ATOM ATOM	428	CA	SER	55	3.240	22.335	4.357	1.00	6.86
ATOM	430	CB	SER	55	1.916	22.675	3.694	1.00	7.85
ATOM	431	OG	SER	55	0.981	23.194	4.615	1.00	11.52
ATOM	432	c	SER	55	3.098	21.410	5.563	1.00	6.98
ATOM	433	0	SER	5 5	3.081	21.834	6.713	1.00	7.09
ATOM	434	N	GLN	56	2.961	20.107	5.309	1.00	7.22

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ATOM	435	CA	GLN	56	2.784	19.139	6.379	1.00	7 20
ATOM	436	CB	GLN	56	2.400	17.785	5.799	1.00	7.20 9.23
ATOM	437	CG	GLN	56	2.329	16.657	6.795	1.00	11.52
ATOM	438	CD	GLN	56	1.214	16.804	7.803	1.00	14.79
ATOM ATOM	439 440	OE1 NE2	GLN	56	1.405	16.302	8.912	1.00	22.67
ATOM	441	C C	GLN GLN	56 56	0.122	17.443	7.423	1.00	13.58
ATOM	442	0	GLN	56	4.007	19.101 19.099	7.279	1.00	7.77
ATOM	443	N	LYS	57	5.188	18.978	8.517 6.684	1.00	7.98
ATOM	444	CA	LYS	57	6.404	18.904	7.465	1.00 1.00	6.97
ATOM	445	CB	LYS	57	7.622	18.583	6.598	1.00	7.11
ATOM	446	CG	LYS	57	7.574	17.249	5.861	1.00	7.89 7.92
ATOM	447	CD	LYS	57	7.561	16.023	6.784	1.00	9.42
ATOM	448	CE	LYS	57	7.650	14.765	5.962	1.00	10.57
ATOM ATOM	449	NZ	LYS	57	7.444	13.524	6.770	1.00	13.31
ATOM	450 451	c o	LYS LYS	57	6.623	20.175	8.273	1.00	6.73
ATOM	452	N	THR	57 58	7.102 6.325	20.149	9.413	1.00	8.29
ATOM	453	CA	THR	58	6.448	21.322 22.618	7.676	1.00	7.11
ATOM	454	CB	THR	58	6.257	23.767	8.342 7.355	1.00	7.21
MOTA	455	0G1	THR	58	7.318	23.725	6.392	1.00 1.00	7.45
ATOM	45 <i>6</i>	CG2	THR	56	6.316	25.134	8.054	1.00	8.22 8.05
ATOM	457	С	THR	58	5.495	22.727	9.527	1.00	6.99
MOTA	458	0	THR	58	5.879	23.194	10.618	1.00	7.76
ATOM	459	N	LYS	59	4.257	22.255	9.336	1.00	7.98
ATOM ATOM	460 461	CA	LYS	59	3.270	22.244	10.430	1.00	8.41
ATOM	462	CB CG	LYS LYS	59 59	1.933	21.732	9.870	1.00	11.31
ATOM	463	CD	LYS	59 59	0.857 -0.412	21.678 21.032	10.962	1.00	17.36
ATOM	464	CE	LYS	59	-0.145	19.572	10.378 10.080	1.00	21.57
ATOM	465	NZ	LYS	59	0.949	19.018	10.953	1.00 1.00	26.63
ATOM	466	C	LYS	59	3.756	21.375	11.583	1.00	41.28 8.97
ATOM	467	0	LYS	59	3.662	21.789	12.743	1.00	9.25
ATOM	468	N	GLU	60	4.260	20.182	11.254	1.00	8.73
ATOM	469	CA	GLU	60	4.763	19.297	12.288	1.00	9.20
ATOM ATOM	470	CB	GLU	60	5.286	17.988	11.679	1.00	10.60
ATOM	471 472	CG CD	GLU GLU	60	4.189	17.114	11.083	1.00	13.69
ATOM	473	OE1	GLU	60 60	4.634 5.846	15.954	10.241	1.00	15.34
ATOM	474	OE2	GLU	60	3.819	15.700 15.290	10.211 9.550	1.00	20.83
MOTA	475	С	GLU	60	5.849	19.961	13.119	1.00	19.41
ATOM	476	0	GLU	60	5.822	19.898	14.353	1.00	10.04 11.42
ATOM	477	N	PHE	61	6.751	20.687	12.465	1.00	8.91
ATOM	478	CA	PHE	61	7.785	21.443	13.184	1.00	7.35
ATOM ATOM	479	CB	PHE	61	8.775	21.958	12.129	1.00	7.73
ATOM	480 481	CG CD1	PHE	61	9.763	22.977	12.665	1.00	8.40
ATOM	482	CD2	PHE	61	10.749	22.594	13.521	1.00	9.42
ATOM	483	CE1	PHE	61 61	9.667 11.653	24.316 23.520	12.302	1.00	10.73
ATOM	484	CE2	PHE	61	10.591	25.256	13.994 12.727	1.00	10.45
ATOM	485	CZ	PHE	61	11.562	24.834	13.606	1.00	11.37
ATOM	486	С	PHE	61	7.211	22.579	14.015	1.00	10.57 7.60
ATOM	487	0	PHE	61	7.474	22.658	15.228	1.00	8.53
ATOM	488	N	HIS	62	6.446	23.487	13.426	1.00	8.25
ATOM	489	CA	HIS	62	5.921	24.635	14.156	1.00	8.66
ATOM ATOM	490 491	CB	HIS	62	5.076	25.531	13.261	1.00	9.03
ATOM	492	CG CD2	HIS HIS	62 62	5.800	26.423	12.311	1.00	8.36
ATOM	493	ND1	HIS	62	5.271 6.963	26.774	11.094	1.00	7.90
ATOM	494	CE1	HIS	62	7.123	27.124 27.845	12.415 11.303	1.00	10.22
ATOM	495	NE2	HIS	62	6.122	27.622	10.488	1.00	7.76
ATOM	496	С	HIS	62	5.091	24.264	15.385	1.00	10.59 9.71
ATOM	497	0	HIS	62	5.070	24.974	16.376	1.00	11.19
ATOM	498	N	MET	63	4.335	23.167	15.283	1.00	10.41
ATOM	499	CA	MET	63	3.393	22.836	16.321	1.00	12.27
ATOM ATOM	500	CB	MET	63	2.151	22.162	15.705	1.00	13.32
ATOM	501 502	CG SD	MET	63	1.453	23.061	14.692	1.00	14.13
ATOM	502	CE	MET MET	63 63	1.062	24.757	15.253	1.00	21.44
ATOM	504	C	MET	63	0.528 4.020	25.519 22.008	13.715	1.00	41.15
ATOM	505	0	MET	63	3.383	22.008	17.416 18.470	1.00	13.21
ATOM	506	И .	SER	64	5.203	21.457	17.178	1.00 1.00	19.62
ATOM	507	CA	SER	64	5.896	20.662	18.191	1.00	10.61
								2.00	13.44

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ATOM	508	CB	SER	64	6.289	19.283	17.662	1.00	15.70
ATOM	509	OG	SER	64	7.299	19.356	16.689	1.00	17.37
ATOM	510	С	SER	64	7.105	21.342	18.809	1.00	12.71
ATOM	511	0	SER	64	7.528	20.933	19.888	1.00	16.31 10.13
ATOM	512	И	ILE	65	7.664	22.392	18.236 18.900	1.00 1.00	9.79
ATOM	513	CA	ILE	65	8.799	23.010 23.968	17.906	1.00	10.92
MOTA	514	CB	ILE ILE	65 65	9.469 8.583	25.072	17.406	1.00	13.10
ATOM	515	CG2 CG1	ILE	65	10.787	24.455	18.502	1.00	11.85
ATOM	516 517	CD1	ILE	65	11.740	25.156	17.598	1.00	13.44
ATOM ATOM	518	C	ILE	65	8.366	23.703	20.162	1.00	10.18
ATOM	519	0	ILE	65	7.286	24.267	20.263	1.00	12.62
ATOM	520	N	THR	66	9.170	23.608	21.194	1.00	10.22
ATOM	521	CA	THR	66	8.866	24.106	22.535	1.00	10.08
MOTA	522	CB	THR	66	9.278	23.065	23.583	1.00 1.00	9.9 7 12.07
MOTA	523	OG1	THR	66	10.681	22.892	23.511 23.373	1.00	14.54
MOTA	524	CG2	THR	66	8.571	21.749 25.420	22.846	1.00	8.74
ATOM	525	C	THR	66 66	9.559 10.531	25.775	22.160	1.00	8.66
ATOM	526	N	THR PRO	67	9.078	26.142	23.864	1.00	9.12
ATOM	527 528	CD	PRO	67	7.813	25.938	24.594	1.00	11.31
ATOM ATOM	529	CA	PRO	67	9.724	27.392	24.251	1.00	9.65
ATOM	530	CB	PRO	67	8.925	27.860	25.450	1.00	12.19
ATOM	531	CG	PRO	67	7.598	27.233	25.312	1.00	12.99
ATOM	532	C	PRO	67	11.209	27.228	24.567	1.00	9.34 10.59
ATOM	533	0	PRO	67	12.046	28.064	24.200	1.00	10.59
ATOM	534	N	GLU	68	11.597	26.115	25.186 25.470	1.00 1.00	11.64
ATOM	535	CA	GLU	68	13.000	25.861 24.533	26.244	1.00	13.13
MOTA	536	CB	GLU	68 68	13.061 14.452	24.123	26.600	1.00	14.22
ATOM	537	CG CD	GLU GLU	68	14.498	22.689	27.107	1.00	15.39
MOTA	538 539	OE1	GLU	68	13.945	21.743	26.508	1.00	21.01
ATOM ATOM	540	OE2	GLU	68	15.043	22.449	28.180	1.00	19.65
ATOM	541	C	GLU	68	13.836	25.799	24.217	1.00	9.32
ATOM	542	0	GLU	68	14.920	26.376	24.096	1.00	11.18
ATOM	543	N	GLU	69	13.319	25.065	23.221	1.00	8.89
ATOM	544	CA	GLU	69	14.015	24.920	21.929	1.00 1.00	9.17 9.44
MOTA	545	CB	GLU	69	13.310	23.921	21.010 21.576	1.00	10.83
ATOM	546	CG	GLU	69	13.338	22.513 21.627	20.745	1.00	12.92
ATOM	547	CD	GLU	69 69	12.432 12.996	20.941	19.876	1.00	19.22
ATOM	548	OE1 OE2	GLU GLU	69	11.213	21.599	21.003	1.00	19.62
ATOM	549 550	C C	GLU	69	14.157	26.247	21.213	1.00	8.87
ATOM ATOM	551	0	GLU	69	15.153	26.521	20.573	1.00	9.17
ATOM	552	N	LYS	70	13.126	27.086	21.311	1.00	8.65
ATOM	553	CA	LYS	70	13.148	28.387	20.621	1.00	8.41
MOTA	554	CB	LYS	70	11.786	29.100	20.695	1.00	8.73 8.40
ATOM	555	CG	LYS	70	10.663	28.358	19.977	1.00 1.00	9.16
MOTA	556	CD	LYS	70	9.319	29.001	20.239 19. 7 26	1.00	10.86
ATOM	557	CE	LYS	70	8.198 6.875	28.102 28.741	19.726	1.00	12.00
MOTA	558	NZ	LYS	70 70	14.268	29.257	21.182	1.00	7.77
ATOM	559	С	LYS LYS	70	14.992	29.885	20.400	1.00	8.10
ATOM	560 561	O N	TRP	71	14.418	29.325	22.514	1.00	7.55
ATOM ATOM	562	CA	TRP	71	15.556	30.080	23.057	1.00	7.86
ATOM	563	CB	TRP	71	15.545	30.104	24.582	1.00	8.53
ATOM	564	CG	TRP	71	14.467	30.932	25.195	1.00	7.80
ATOM	565	CD2	TRP	71	14.216	32.335	25.045	1.00	7.55
MOTA	566	CE2	TRP	71	13.097	32.672	25.824	1.00	8.56 8.26
ATOM	567	CE3	TRP	71	14.813	33.362	24.326	1.00 1.00	8.54
MOTA	568	CD1		71	13.512	30.477	26.068 26.446	1.00	9.24
MOTA	569	NEl				31.521 33.965	25.900	1.00	9.23
MOTA	570	CZ2		71 71		34.644	24.384	1.00	8.95
ATOM	571	CZ3		71		34.947	25.181	1.00	9.37
ATOM	572 573	CH2 C	TRP	71		29.513	22.565	1.00	7.41
ATOM	573 574	0	TRP	71		30.271	22.223	1.00	7.75
ATOM ATOM	574 575	И	ASP	72		28.180	22.552	1.00	7.95
ATOM	576	CA	ASP	72		27.508	22.215	1.00	9.24
ATOM	577	CB	ASP	72		26.031	22.638	1.00	11.24
ATOM	578	CG	ASP	. 72		25.822	24.146	1.00	14.08
ATOM	579	OD1		72		26.778	24.967	1.00	15.23 17.93
ATOM	580	OD2	ASP	72	17.942	24.678	24.599	1.00	11.53

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ATOM	581	С	ASP	7	2 18.589	27.715	20. 26.		
ATOM	582	0	ASP	7			20.764	1.00	9.14
ATOM	583	N	LEU	7		27.980	20.413	1.00	10.16
ATOM	584	CA	LEU	7.		28.233	19.872	1.00	7.62
ATOM	585	CB	LEU	7		27.452	18.474	1.00	8.24
ATOM	586	CG		7		25.941	17.648	1.00	9.44
ATOM	587	CD		7:		25.238	17.683	1.00	10.93
MOTA	589	CD:		7:	_		17.093	1.00	16.41
ATOM	589	С	LEU	73		25.437	17.077	1.00	14.97
ATOM	590	o	LEU	73		29.708	18.102	1.00	7.12
ATOM	591	N	ALA	74		30.074	16.935	1.00	7.82
ATOM	592	CA	ALA	74		30.607	19.036	1.00	6.72
ATOM	593	СВ	ALA	74		31.967	18.766	1.00	6.46
ATOM	594	c	ALA	74		32.662	20.042	1.00	7.96
ATOM	595	ō	ALA	74		32.818	18.098	1.00	7.50
ATOM	596	N	ILE			32.697	18.490	1.00	8.38
ATOM	597	CA	ILE	75		33.689	17.172	1.00	6.76
ATOM	598	CB	ILE	75		34.680	16.652	1.00	6.71
ATOM	599	CG2		75		35.376	15.420	1.00	6.88
MOTA	600	CG1		75		34.424	14.239	1.00	8.21
MOTA	601	CD1		75 		36.140	15.755	1.00	7.17
ATOM	602			75 	16.522	37.151	14.715	1.00	9.71
ATOM	603	C	ILE	75	19.201	35.704	17.734	1.00	7.09
ATOM		0	ILE	75	18.546	35.810	18.781	1.00	6.89
ATOM	604	N	ALA	76	20.280	36.421	17.461	1.00	8.25
ATOM	605	CA	ALA	76	20.876	37.407	18.360	1.00	9.65
ATOM	606	CB	ALA	76	22.084	38.067	17.666	1.00	16.12
	607	C	ALA	76	19.886	38.445	18.838	1.00	8.48
ATOM	608	0	ALA	76	19.962	38.940	19.953	1.00	9.39
ATOM	609	N	ALA	77	18.905	38.810	18.002	1.00	
ATOM	610	CA	ALA	77	17.911	39.8 0 0	18.374	1.00	8.30
ATOM	611	CB	ALA	77	16.992	40.064	17.179	1.00	9.45
ATOM	612	С	ALA	77	17.100	39.352	19.582		10.84
ATOM	613	0	ALA	77	16.541	40.191	20.299	1.00	8.44
ATOM	614	N	TYR	78	16.967	38.049	19.816	1.00	10.71
ATOM	6 1 5	CA	TYR	78	16.222	37.513	20.938	1.00	7.56
ATOM	616	CB	TYR	78	15.223	36.420	20.451	1.00	8.24
ATOM	617	CG	TYR	78	14.158	37.043		1.00	7.69
ATOM	618	CD1	TYR	78	14.272	36.972	19.575	1.00	7.53
ATOM	619	CE1	TYR	78	13.370	37.508	18.193	1.00	7.61
ATOM	620	CD2	TYR	78	13.050		17.335	1.00	7.49
ATOM	621	CE2	TYR	78	12.150	37.728	20.079	1.00	8.66
ATOM	622	CZ	TYR	78	12.291	38.290	19.216	1.00	9.02
ATOM	623	ОН	TYR	78	11.357	38.173	17.845	1.00	8.23
ATOM	624	C	TYR	78	17.115	38.805	17.028	1.00	10.37
ATOM	625	0	TYR	78		36.920	22.016	1.00	7.16
ATOM	626	N	ASN	79	16.681	36.716	23.134	1.00	10.37
ATOM	627	CA	ASN	79	18.346	36.542	21.694	1.00	8.52
ATOM	628	CB	ASN		19.232	35.854	22.624	1.00	7.53
ATOM	629	CG	ASN	79 70	19.164	34.338	22.379	1.00	7.59
ATOM	630	OD1		79	20.000	33.518	23.343	1.00	7.82
ATOM	631		ASN	79	20.942	34.010	23.962	1.00	8.62
ATOM	632	ND2	ASN	79	19.686	32.222	23.477	1.00	9.18
ATOM	633	C	ASN	79	20.653	36.401	22.394	1.00	8.94
ATOM		0	ASN	79	21.341	36.042	21.442	1.00	10.00
ATOM	634	N	LYS	80	21.086	37.226	23.348	1.00	9.67
ATOM	635	CA	LYS	80	22.403	37.853	23.279	1.00	11.21
ATOM	636	CB	LYS	80	22.575	38.808	24.473	1.00	14.70
	637	CG	LYS	80	21.697	40.035	24.385	1.00	
ATOM	638	CD	LYS	80	21.970	41.007	25.532	1.00	20.93
ATOM	639	CE	LYS	80	21.540	42.420	25.219	1.00	25.64
ATOM	640	NZ	LYS	80	20.209	42.711	25.795	1.00	29.22
ATOM	641	С	LYS	80	23.565	36.877	23.274	1.00	39.86
ATOM	642	0	LYS	80	24.702	37.192	22.944		10.80
ATOM	643	N	GLU	81	23.349	35.630	23.706	1.00 1.00	13.45
ATOM	644	CA	GLU	81	24.436	34.666	23.722		10.06
ATOM	645	CB	GLU	81	24.060	33.385	24.505	1.00	11.25
MOTA	646	CG	GLU	81	23.668	33.565		1.00	11.80
ATOM	647	CD	GLU	81	23.394	32.322	25.948	1.00	15.18
ATOM	648	OE1	GLU	81	22.810	32.322	26.768	1.00	16.40
ATOM	649	OE2	GLU	81	23.688	31.185	27.889	1.00	16.96
ATOM	650	С	GLU	81	24.791		26.315	1.00	21.03
ATOM	651	o	GLU	81	25.838	34.265	22.281	1.00	12.20
ATOM	652	N .	HIS	82	23.900	33.655	22.069	1.00	14.12
ATOM	653	CA	HIS	82	24.112	34.439	21.316	1.00	10.21
			•			33.865	19.980	1.00	9.63

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				0.0	22.803	33.231	19.530	1.00	9.27
ATOM	654		HIS		22.803	32.070	20.360	1.00	9.26
MOTA	655		HIS		23.068	31.323	21.257	1.00	10.67
MOTA	656		HIS HIS		21.113	31.516	20.288	1.00	8.55
MOTA	657		HIS	82	21.063	30.500	21.141	1.00	8.43
MOTA	658		HIS	82	22.223	30.366	21.742	1.00	10.55
ATOM	659		HIS	82	24.567	34.933	19.029	1.00	10.23
MOTA	660 661		HIS	82	23.901	35.266	18.055	1.00	11.36
ATOM	662		GLN	83	25.726	35.507	19.295	1.00	12.56
ATOM	663		GLN	83	26.203	36.634	18.507	1.00	13.52 16.22
ATOM ATOM	664		GLN	83	27.470	37.164	19.181	1.00	19.23
ATOM	665	CG	GLN	83	27.163	37.925	20.478	1.00 1.00	20.38
ATOM	666	CD	GLN	83	26.294	39.148	20.300	1.00	29.81
ATOM	667	OE1	GLN	83	26.558	40.074	19.536 21.046	1.00	22.46
ATOM	668	NE2	GLN	83	25.191	39.208	17.050	1.00	13.44
ATOM	669	C	GLN	83	26.450	36.332	16.246	1.00	15.10
ATOM	670	0	GLN	83	26.392	37.262	16.694	1.00	13.17
MOTA	671	N	ASP	84	26.636	35.089 34.722	15.292	1.00	14.01
MOTA	672	CA	ASP	84	26.862	33.451	15.162	1.00	17.37
MOTA	673	CB	ASP	84	27.692 29.128	33.607	15.603	1.00	20.70
MOTA	674	CG	ASP	84	29.618	34.762	15.567	1.00	24.40
MOTA	675	OD1	ASP	84 84	29.754	32.593	15.997	1.00	26.32
MOTA	676	OD2	ASP	84	25.612	34.566	14.450	1.00	13.94
MOTA	677	C	ASP	84	25.668	34.506	13.229	1.00	13.72
MOTA	678	0	ASP GLN	85	24.472	34.468	15.125	1.00	12.76
MOTA	679	N CA	GLN	85	23.186	34.270	14.473	1.00	11.48
ATOM	680 681	CB	GLN	85	22.324	33.390	15.381	1.00	11.21
ATOM	682	CG	GLN	85	22.791	31.971	15.552	1.00	11.91
ATOM	683	CD	GLN	85	21.795	31.109	16.278	1.00	10.83
MOTA	684	OE1	GLN	85	20.636	30.970	15.841	1.00	12.23 9.17
ATOM	685	NE2	GLN	85	22.225	30.557	17.380	1.00	12.01
ATOM	686	C	GLN	85	22.468	35.584	14.216	1.00	14.96
MOTA MOTA	687	0	GLN	85	21.590	36.041	14.977	1.00	10.72
ATOM	688	N	VAL	86	22.773	36.203	13.091	1.00 1.00	11.56
ATOM	689	CA	VAL	86	22.062	37.392	12.684	1.00	12.29
ATOM	690	CB	VAL	86	23.031	38.325	11.951	1.00	16.28
MOTA	691	CG1	VAL	86	22.341	39.541	11.368 12.807	1.00	17.21
MOTA	692	CG2	VAL	86	24.227	38.725	11.853	1.00	11.74
ATOM	693	С	VAL	86	20.862	36.994	12.126	1.00	17.43
ATOM	694	0	VAL	86	19.737	37.435	10.898	1.00	8.59
MOTA	695	N	ARG	87	21.060	36.084 35.624	9.972	1.00	7.72
MOTA	696	CA	ARG	87	20.044	35.441	8.553	1.00	8.11
MOTA	697	CB	ARG	87		36.706	7.959	1.00	8.47
ATOM	698	CG	ARG	87 87		36.462	6.599	1.00	7.75
MOTA	699	CD	ARG	87		36.173	5.609	1.00	7.39
ATOM	700	NE	ARG	87		35.691	4.396	1.00	6.65
MOTA	701	CZ	ARG ARG	87		35.389	3.959	1.00	8.68
MOTA	702	NH1 NH2	ARG	87		35.471	3.547	1.00	7.51
ATOM	703 704	C	ARG	87		34.289	10.332	1.00	7.27
ATOM	704	0	ARG	87		34.129	10.237	1.00	8.33 7.40
ATOM	706	N	ALA	88	20.206	33.270	10.609	1.00	6.92
MOTA	707	CA	ALA	88	19.749	3 1 . 8 76	10.750	1.00	8.59
MOTA MOTA	708	СВ	ALA	88	3 20.760	30.869	10.254	1.00 1.00	7.06
ATOM	709	С	ALA	88		31.526	12.165	1.00	9.57
ATOM	710	0	ALA	88		31.793	13.084	1.00	6.44
ATOM	711	N	GLY	8		30.953	12.332 13.592	1.00	6.74
ATOM	712	CA	GLY	8		30.494	13.801	1.00	6.23
MOTA	713	C	GLY	8			12.853	1.00	6.32
ATOM	714	0	GLY		9 15.451		15.062	1.00	6.31
MOTA	715	N	TYR		0 15.811		15.460	1.00	6.71
ATOM	716	CA	TYR		0 14.439		16.623	1.00	7.29
ATOM	717	СВ	TYR		0 14.009		16.487	1.00	6.81
ATOM	718	CG	TYR		0 12.552		15.755	1.00	7.89
MOTA	719				0 12.151		15.592	1.00	8.96
MOTA	720				0 10.830		17.042	1.00	7.06
MOTA	721				90 11.536 90 10.193		16.837	1.00	8.48
MOTA	722						16.124	1.00	9.10
MOTA	723						051	1.00	13.43
ATOM	724				90 8.559 90 14.19			1.00	6.30
MOTA	725		TYR		90 14.198			1.00	6.78
MOTA	726	. 0	TYR						

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	PCT/GB97	7/02838
15.320	1.00	6.07
15.484	1.00	6.47
14.135	1.00	6.78

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	727	N	TYR	91	13.035	33.030	15.320	1.00	6.07
ATOM ATOM	727	CA	TYR	91	12.554	34.384	15.484	1.00	6.47 6.78
ATOM	729	СВ	TYR	91	12.252	35.025	14.135 13.209	1.00 1.00	6.23
ATOM	730	CG	TYR	91	13.392	35.277 34.332	12.859	1.00	7.06
ATOM	731	CD1	TYR	91	14.353	34.332	11.962	1.00	7.29
ATOM	732	CE1	TYR	91	15.364 13.490	36.521	12.556	1.00	7.46
ATOM	733	CD2	TYR	91 91	14.486	36.776	11.634	1.00	7.96
ATOM	734	CE2 CZ	TYR TYR	91	15.428	35.826	11.343	1.00	6.61
MOTA	735 736	OH	TYR	91	16.438	36.143	10.440	1.00	8.55
ATOM	737	C	TYR	91	11.289	34.262	16.334	1.00	5.71
ATOM ATOM	738	o	TYR	91	10.273	33.788	15.843	1.00	6.82 6.69
ATOM	739	N	LEU	92	11.385	34.619	17.619 18.569	1.00	6.33
ATOM	740	CA	LEU	92	10.306	34.337 34.371	19.987	1.00	7.20
ATOM	741	CB	LEU	92	10.873	33.188	20.466	1.00	7.89
ATOM	742	CG	LEU	92 92	11.700 13.022	33.165	19.735	1.00	8.67
ATOM	743	CD1	LEU	92	11.888	33.261	21.985	1.00	10.35
ATOM	744	CD2	LEU	92	9.151	35.317	18.471	1.00	6.37
MOTA	745 746	C 0	LEU	92	9.284	36.491	18.161	1.00	7.36
ATOM	747	N	SER	93	7.976	34.786	18.810	1.00	7.12 7.59
MOTA MOTA	748	CA	SER	93	6.805	35.605	19.060	1.00	8.96
ATOM	749	СВ	SER	93	5.523	34.794	19.013 20.074	1.00	11.17
ATOM	750	QG	SER	93	5.410	33.894	20.074	1.00	7.83
ATOM	751	C	SER	93	6.928	36.224 35.807	21.266	1.00	8.58
ATOM	752	0	SER	93	7.728 6.100	37.213	20.688	1.00	9.38
MOTA	753	N	ILE	94 94	6.029	37.865	22.016	1.00	9.91
MOTA	754	CA	ILE ILE	94	6.640	39.280	21.992	1.00	10.58
MOTA	755 756	CB CG2	ILE	94	6.575	39.842	23.385	1.00	11.13
ATOM	756 757	CG1	ILE	94	8.051	39.304	21.385	1.00	11.02 12.81
ATOM ATOM	758	CD1	ILE	94	8.740	40.630	21.225	1.00 1.00	9.85
ATOM	759	С	ILE	94	4.550	37.947	22.376 21.906	1.00	11.19
ATOM	760	0	ILE	94	3.881	38.887	23.046	1.00	10.93
ATOM	761	N	PRO	95	4.006	36.948 35.749	23.520	1.00	12.42
MOTA	762	CD	PRO	95	4.693 2.560	36.878	23.342	1.00	12.23
MOTA	763	CA	PRO	95 9 5	2.394	35.670	24.234	1.00	13.83
MOTA	764	CB	PRO PRO	95	3.555	34.807	23.867	1.00	13.55
ATOM	765	CG C	PRO	95	2.064	38.173	23.973	1.00	11.65
ATOM	766 767	0	PRO	95	2.791	38.800	24.780	1.00	12.20 12.67
ATOM ATOM	768	N	GLY	96	0.973	38.667	23.409	1.00	13.37
ATOM	769	CA	GLY	96		39.965	23. 79 9 22.976	1.00	12.23
MOTA	770	С	GLY	96	_	41.142 42.233	23.105	1.00	15.48
MOTA	771	0	GLY	96		40.975	22.189	1.00	12.23
MOTA	772	N	LYS	97		42.048	21.444	1.00	11.30
MOTA	773	CA	LYS	97 97		42.410	22.187	1.00	12.24
MOTA	774	CB CG	LYS LYS	97		42.828	23.625	1.00	13.52
ATOM	7 7 5 7 7 6	CD	LYS	97		44.147	23.758	1.00	15.77
ATOM ATOM	777	CE	LYS	97	3.019	44.549	25.226	1.00	18.45 21.87
ATOM	778	NZ	LYS	97		45.715	25.339	1.00 1.00	10.88
ATOM	779	C	LYS	97		41.783	19.977 19.081	1.00	11.92
MOTA	780	0	LYS	91		42.638 40.583	19.691	1.00	10.38
ATOM	781	N	LYS	98		40.149	18.374	1.00	9.59
ATOM	782	CA	LYS	98		40.215	18.332	1.00	12.06
ATOM	783	CB	LYS	9:	-	39.618	17.105	1.00	11.30
ATOM	784	CG	LYS LYS	9		39.879	17.116	1.00	10.99
MOTA	785	CD	LYS	9		39.370	15.908	1.00	10.76
MOTA	786 787	NZ	LYS	9		37.856	15.937	1.00	10.00 9.52
ATOM	788	C	LYS		8 3.462	38.723	18.145	1.00	10.44
ATOM ATOM	789	0	LYS	9	8 3.835	37.797	18.884	1.00 1.00	8.69
ATOM	790	N	ALA	9	9 2.674	38.529	17.108	1.00	8.30
ATOM	791	CA	ALA		9 2.095		16.865 16.107	1.00	11.01
ATOM	792	CB			0.771		16.107	1.00	7.09
ATOM	793	С	ALA		9 2.993		16.291	1.00	8.34
ATOM	794	0	ALA		9 3.091			1.00	7.33
ATOM	795		VAL		00 3.614			1.00	7.31
ATOM	796				00 4.390 00 4.804			1.00	8.26
MOTA	797				00 5.854			1.00	9.84
ATOM	798				00 5.29			1.00	9.08
MOTA	799	C	نهم∨ عد						

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ATOM	800	C	VAL	100		35.463	14.759	1.00	6.77
ATOM ATOM	801	0	VAL	100		36.069	15.614	1.00	6.24
ATOM	902 803	N	GLU	101		34.294	14.261	1.00	5.93
ATOM	804	CA CB	GLU GLU	101 101	=	33.647	14.643	1.00	5.89
ATOM	805	CG	GLU	101		32.758	15.864	1.00	6.83
ATOM	806	CD	GLU	101		31.599 30.900	15.714	1.00	9.01
ATOM	807	OE1		101		31.171	17.058 17.727	1.00	11.15
ATOM	808	OE2	GLU	101		30.033	17.396	1.00 1.00	11.35
ATOM	809	C	GLU	101	7.748	32.835	13.441	1.00	16.56 6.12
ATOM ATOM	810	0	GLU	101	6.989	32.513	12.532	1.00	6.44
ATOM	811 812	N	SER	102	9.047	32.564	13.384	1.00	6.02
ATOM	813	CA CB	SER SER	102	9.605	31.897	12.196	1.00	6.00
ATOM	814	OG	SER	102 102	9.725 10.632	32.906 33.935	11.058	1.00	6.77
ATOM	815	С	SER	102	10.934	31.253	11.388 12.468	1.00	7.64
ATOM	816	0	SER	102	11.592	31.497	13.474	1.00 1.00	6.15
ATOM	817	N	PHE	103	11.367	30.433	11.517	1.00	6.61 5.73
ATOM	818	CA	PHE	103	12.670	29.792	11.506	1.00	5.88
ATOM ATOM	819	CB	PHE	103	12.521	28.294	11.756	1.00	6.37
ATOM	820 821	CG CD1	PHE	103	13.795	27.476	11.663	1.00	6.21
ATOM	822	CD1	PHE PHE	103 103	14.723	27.499	12.686	1.00	7.53
ATOM	823	CE1	PHE	103	14.034 15.866	26.650	10.562	1.00	7.03
ATOM	824	CE2	PHE	103	15.167	26.713 25.887	12.620	1.00	7.78
ATOM	825	CZ	PHE	103	16.077	25.924	10.483 11.508	1.00	6.93
MOTA	826	C	PHE	103	13.319	30.018	10.149	1.00	7.07
ATOM	827	0	PHE	103	12.720	29.679	9.124	1.00	5.84 5.89
ATOM	828	N	CYS	104	14.505	30.596	10.128	1.00	5.38
ATOM ATOM	829	CA	CYS	104	15.244	30.888	8.907	1.00	5.34
ATOM	830 831	CB SG	CYS	104	15.669	32.368	8.935	1.00	6.38
ATOM	832	C	CYS CYS	104 104	16.693 16.475	32.902	7.544	1.00	7.14
ATOM	833	ō	CYS	104	17.202	29.988 29.801	8.802	1.00	5.05
ATOM	834	N	TYR	105	16.758	29.512	9. 7 94 7.6 1 5	1.00	5.55
ATOM	835	CA	TYR	105	17.979	28.794	7.344	1.00	5.01
ATOM	836	CB	TYR	105	17.839	27.285	7.499	1.00	4.98 5.67
ATOM	837	CG	TYR	105	16.822	26.594	6.589	1.00	5.07
ATOM ATOM	838	CD1	TYR	105	17.258	25.856	5.491	1.00	5.34
ATOM	839 840	CE1 CD2	TYR TYR	105	16.371	25.171	4.659	1.00	5.87
ATOM	841	CE2	TYR	105 105	15.469 14.595	26.551	6.883	1.00	5.19
ATOM	842	CZ	TYR	105	15.045	25.862 25.169	6.059	1.00	5.89
MOTA	843	ОН	TYR	105	14.141	24.495	4.966 4.169	1.00	5.38
ATOM	844	C	TYR	105	18.515	29.202	5.972	1.00	6.39
ATOM	845	0	TYR	105	17.778	29.622	5.072	1.00	4.38 5.26
ATOM ATOM	846	N	LEU	106	19.816	29.039	5.852	1.00	5.00
ATOM	847 848	CA	LEU	106	20.634	29.415	4.731	1.00	4.93
ATOM	849	CB CG	LEU LEU	106 106	21.803	30.266	5.227	1.00	6.26
ATOM	850	CD1	LEU	106	21.444 22.709	31.467	6.125	1.00	6.45
ATOM	851	CD2	LEU	106	20.392	32.219 32.329	6.477	1.00	8.37
ATOM	852	С	LEU	106	21.121	28.188	5.466 3.948	1.00	6.90
ATOM	853	0	LEU	106	20.754	27.046	4.237	1.00	4.77 5.93
ATOM	854	N	ASN	107	21.991	28.473	2.983	1.00	4.96
ATOM ATOM	855	CA	ASN	107	22.654	27.437	2.187	1.00	5.23
ATOM	856 857	CB	ASN	107	23.803	28.147	1.434	1.00	5.83
ATOM	858	CG OD1	ASN ASN	107 107	24.424	27.280	0.353	1.00	5.32
ATOM	859	ND2	ASN	107	24.420 24.989	26.044	0.396	1.00	5.91
ATOM	860	C	ASN	107	23.225	27.988 26.347	-0.626	1.00	6.49
MOTA	861	0	ASN	107	24.097	26.593	3.079 3.937	1.00	4.82
ATOM	862	N	PRO	108	22.771	25.095	2.881	1.00	5.62
ATOM	863	CD	PRO	108	21.595	24.677	2.118	1.00	4.96 5.43
ATOM	864	CA	PRO	108	23.345	23.973	3.639	1.00	5.82
ATOM	865	CB	PRO	108	22.516	22.773	3.134	1.00	6.84
ATOM ATOM	866 867	CG	PRO	108	21.194	23.377	2.749	1.00	6.32
ATOM	867 868	С 0	PRO	108	24.846	23.763	3.444	1.00	5.93
ATOM	869	И	PRO ASN	108 109	25.533	23.129	4.274	1.00	6.51
ATOM	870	CA	ASN	109	25.397 26.823	24.277	2.353	1.00	5.53
ATOM	871	CB .	ASN	109	26.823	24.180	2.080	1.00	5.84
ATOM	872	CG	ASN	109	26.633	24.369 23.186	0.598 -0.200	1.00	6.10
						-2.100	5.200	1.00	5.51

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ATOM	873	OD1	ASN	109	26.690	22.020	0.209	1.00	7.43
ATOM	874	ND2	ASN	109	26.165	23.491	-1.405	1.00	7.14
ATOM	875	С	ASN	109	27.652	25.150	2.920	1.00	5.95
ATOM	876	0	NSA	109	28.863	25.063	2.911	1.00	6.60 6.52
ATOM	877	N	PHE	110	27.032	26.060	3.672 4.602	1.00 1.00	6.64
MOTA	878	CA	PHE	110	27.727	26.943 28.235	4.934	1.00	6.86
ATOM	879	CB	PHE	110	26.984 26.793	29.203	3.781	1.00	6.62
MOTA	880	CG	PHE PHE	110 110	27.454	29.100	2.593	1.00	6.42
ATOM	881 882	CD1 CD2	PHE	110	25.889	30.238	3.919	1.00	7.13
ATOM ATOM	883	CE1	PHE	110	27.269	30.020	1.570	1.00	7.97
ATOM	884	CE2	PHE	110	25.698	31.178	2.917	1.00	7.73
ATOM	885	CZ	PHE	110	26.380	31.064	1.723	1.00	7.68
ATOM	886	С	PHE	110	28.010	26.131	5.870	1.00	6.41
ATOM	887	0	PHE	110	27.334	26.222	6.890	1.00	9.08 7.20
ATOM	888	N	THR	111	29.047	25.319	5.795	1.00	7.20
MOTA	889	CA	THR	111	29.543	24.473	6.858 6.240	1.00	9.61
ATOM	890	CB	THR	111	29.986	23.114 23.407	5.150	1.00	12.08
ATOM	891	OG1	THR	111	30.863 28.831	22.332	5.660	1.00	11.21
ATOM	892	CG2	THR THR	111 111	30.719	25.173	7.535	1.00	8.55
ATOM	893	С 0	THR	111	31.262	26.161	7.039	1.00	8.43
ATOM	894 895	N	PRO	112	31.158	24.669	8.690	1.00	10.82
ATOM	896	CD	PRO	112	30.500	23.646	9.514	1.00	12.34
ATOM ATOM	897	CA	PRO	112	32.284	25.317	9.365	1.00	10.76
ATOM	898	CB	PRO	112	32.454	24.403	10.591	1.00	12.53
ATOM	899	CG	PRO	112	31.035	23.971	10.884	1.00	13.67
ATOM	900	С	PRO	112	33.560	25.453	8.553	1.00	10.13
ATOM	901	0	PRO	112	34.293	26.449	8.719	1.00	12.02
ATOM	902	N	ASP	113	33.764	24.577	7.586	1.00	10.28
MOTA	903	CA	ASP	113	34.960	24.594	6.754	1.00 1.00	11.85 14.15
ATOM	904	CB	ASP	113	35.418	23.179	6.354	1.00	16.88
ATOM	905	CG	ASP	113	34.450	22.335	5. 55 6 5.265	1.00	17.94
MOTA	906	OD1	ASP	113	34.697	21.122	5.120	1.00	18.33
ATOM	907	OD2	ASP	113	33.431	22.903 25.485	5.516	1.00	10.04
MOTA	908	C	ASP	113	34. 77 9 35.695	25.568	4.674	1.00	11.29
MOTA	909	0	ASP	113 114	33.614	26.058	5.256	1.00	8.19
MOTA	910	N CA	HIS HIS	114	33.388	26.853	4.066	1.00	7.72
MOTA	911	CB	HIS	114	31.924	27.234	3.945	1.00	8.19
MOTA MOTA	912 913	CG	HIS	114	31.514	27.896	2.661	1.00	7.35
ATOM	914	CD2	HIS	114	30.786	27.365	1.634	1.00	7.63
ATOM	915	ND1	HIS	114	31.853	29.194	2.350	1.00	7.74
ATOM	916	CE1	HIS	114	31.374	29.423	1.125	1.00	8.63
ATOM	917	NE2	HIS	114	30.698	28.385	0.701	1.00	8.22 7.89
ATOM	918	С	HIS	114	34.263	28.078	4.069	1.00	8.23
ATOM	919	0	HIS	114	34.363	28.705	5.126	1.00 1.00	8.07
ATOM	920	N	PRO	115	34.877	28.447	2.947 1.595	1.00	9.44
MOTA	921	ČD	PRO	115	34.805	27.853 29.586	2.989	1.00	7.97
MOTA	922	CA	PRO	115	35.791	29.638	1.603	1.00	10.29
ATOM	923	CB	PRO	115 115	36.432 36.058	28.363	0.935	1.00	16.51
MOTA	924	CG	PRO PRO	115		30.906	3.451	1.00	8.16
MOTA	925	C	PRO	115		31.749	4.033	1.00	8.89
ATOM	926 927	И	ARG	116		31.156	3.245	1.00	7.57
MOTA MOTA	928	CA	ARG	116		32.366	3.687	1.00	8.05
ATOM	929	CB	ARG	116		32.649	2.831	1.00	9.75
ATOM	930	CG	ARG	116		33.041	1.398	1.00	11.43
ATOM	931	CD	ARG	116	33.024	34.444	1.316	1.00	17.12
ATOM	932	NE ·	ARG	116	32.909	34.976	-0.046	1.00	18.64
ATOM	933	CZ	ARG	116		36.202	-0.332	1.00	16.55 18.90
MOTA	934	NH1	ARG	116		37.005	0.626	1.00	19.38
ATOM	935	NH2	ARG	116		36.628	-1.550	1.00 1.00	8.18
ATOM	936	C	ARG	116		32.353	5.168 5.807	1.00	10.55
ATOM	937	0	ARG	116		33.426	5.702	1.00	7.91
MOTA	938	N	ILE	117		31.161 30.993	7.134	1.00	8.74
ATOM	939	CA	ILE	117		29.617	7.425	1.00	8.27
MOTA	940	CB	ILE	117		29.337	8.920	1.00	10.79
ATOM	941	CG2	ILE	117		29.510	6.798	1.00	7.78
MOTA	942	CG1 CD1		11		30.458	7.376	1.00	9.72
ATOM	943 944	CDI	· ILE	11		31.170	7.818	. 1.00	9.52
ATOM	944	0	ILE	11		31.893	8.820	1.00	10.02
ATOM	242	•							

ATOM	946	N	GLN	118	34.936	30.601	7.248	1.00	9.60
ATOM	947	CA	GLN	118	36.264	30.823	7.814	1.00	9.55
ATOM	948	CB	GLN	119	37.287	29.975	7.066		
ATOM	949	CG	GLN	118	37.163	28.475	7.285	1.00	11.20
ATOM	950	CD	GLN	118	37.706	28.064		1.00	11.87
ATOM	951	OE1	GLN	118			8.628	1.00	15.84
ATOM	952	NE2	GLN		38.799	28.509	9.021	1.00	16.95
ATOM				118	36.968	27.189	9.314	1.00	18.58
	953	C	GLN	118	36.624	32.301	7.782	1.00	10.34
MOTA	954	0	GLN	118	37.209	32.780	8.779	1.00	12.18
ATOM	955	N	ALA	119	36.307	33.008	6.719	1.00	10.58
ATOM	956	CA	ALA	119	36.652	34.437	6.577	1.00	11.17
MOTA	957	CB	ALA	119	36.675	34.884	5.141	1.00	11.90
ATOM	958	C	ALA	119	35.766	35.340	7.417	1.00	11.81
ATOM	959	0	ALA	119	35.975	36.547	7.593	1.00	13.51
ATOM	960	N	LYS	120	34.677	34.792	7.926		
ATOM	961	CA	LYS	120	33.697	35.524		1.00	11.51
ATOM	962	CB	LYS	120			8.728	1.00	11.83
ATOM					34.314	36.156	9.981	1.00	16.43
	963	CG	LYS	120	35.156		10.773	1.00	20.21
ATOM	964	CD	LYS	120	34.452	34.007	11.336	1.00	25.82
MOTA	965	CE	LYS	120	35.422	33.080	12.083	1.00	26.48
ATOM	966	NZ	LYS	120	36.364	32.304	11.194	1.00	23.67
ATOM	967	C	LYS	120	33.033	36.623	7.910	1.00	12.07
MOTA	968	0	LYS	120	32.701	37.698	8.413	1.00	13.32
ATOM	969	N	THR	121	32.773	36.290	6.647	1.00	11.59
ATOM	970	CA	THR	121	32.162	37.294	5.783		
ATOM	971	CB	THR	121	32.158	36.758		1.00	11.41
ATOM	972	OG1	THR	121			4.336	1.00	11.74
ATOM	973	CG2			33.515	36.460	3.947	1.00	14.18
ATOM			THR	121	31.617	37.825	3.394	1.00	13.26
	974	C	THR	121	30.742	37.599	6.199	1.00	10.30
ATOM	975	0	THR	121	30.016	36.627	6.442	1.00	9.38
ATOM	976	N	PRO	122	30.343	38.869	6.255	1.00	11.24
ATOM	977	CD	PRO	122	31.175	40.087	6.162	1.00	13.40
MOTA	978	CA	PRO	122	28.938	39.176	6.605	1.00	10.67
MOTA	979	CB	PRO	122	28.883	40.676	6.374	1.00	13.30
ATOM	980	CG	PRO	122	30.251	41.155	6.684	1.00	14.04
ATOM	981	С	PRO	122	27.933	38.454	5.721	1.00	
ATOM	982	0	PRO	122	28.224	38.174	4.567		8.90
ATOM	983	N	THR	123	26.810			1.00	9.02
ATOM	984	CA	THR	123	25.660	38.105	6.329	1.00	9.47
ATOM						37.447	5.729	1.00	8.42
	985	CE	THR	123	25.112	38.105	4.455	1.00	9.93
ATOM	986	OG1	THR	123	25.929	37.810	3.314	1.00	10.18
ATOM	987	CG2	THR	123	25.024	39.629	4.512	1.00	13.04
ATOM	988	С	THR	123	25.807	35.938	5.560	1.00	8.70
ATOM	989	0	THR	123	24.815	35.273	5.198	1.00	9.15
ATOM	990	N	HIS	124	26.994	35.395	5.833	1.00	8.34
ATOM	991	CA	HIS	124	27.189	33.957	5.798	1.00	7.64
ATOM	992	CB	HIS	124	28.524	33.584	5.149	1.00	7.45
ATOM	993	CG	HIS	124	28.726	34.113	3.780	1.00	7.43
ATOM	994	CD2	HIS	124	28.755	33.507	2.577	1.00	
ATOM	995	ND1	HIS	124	28.998	35.449			7.26
ATOM	996	CE1	HIS	124			3.557	1.00	7.88
ATOM	997				29.202	35.607	2.261	1.00	8.29
		NE2	HIS	124	29.032	34.478	1.631	1.00	7.93
ATOM	998	C	HIS	124	27.170	33.387	7.206	1.00	8.19
MOTA	999	0	HIS	124	27.888	33.913	8.056	1.00	9.17
ATOM	1000	N	GLU	125	26.413	32.313	7.455	1.00	7.36
MOTA	1001	CA	GLU	125	26.337	31.694	8.776	1.00	7.74
ATOM	1002	CB	GLU	125	25.166	32.230	9.604	1.00	8.77
ATOM	1003	CG	GLU	125	25.164	33.714	9.832	1.00	9.78
ATOM	1004	CD	GLU	125	23.885	34.235	10.445	1.00	9.41
ATOM	1005	OE1	GLU	125	23.057	33.439	10.972	1.00	
ATOM	1006	OE2	GLU	125	23.791	35.476			12.02
ATOM	1007	C	GLU	125	26.118		10.373	1.00	12.25
ATOM	1007	0	GLU	125		30.196	8.567	1.00	7.57
ATOM					25.581	29.787	7.521	1.00	8.65
	1009	N	VAL	126	26.505	29.398	9.557	1.00	7.88
MOTA	1010	CA	VAL	126	26.219	27.969	9.636	1.00	7.38
ATOM	1011	CB	VAL	126	27.281	27.246	10.488	1.00	8.22
ATOM	1012	CG1	VAL	126	26.979	25.754	10.561	1.00	9.54
ATOM	1013	CG2	VAL	126	28.686	27.497	9.941	1.00	9.36
ATOM	1014	С	LAV	126	24.843	27.785	10.272	1.00	7.39
ATOM	1015	0	VAL	126	24.564	28.311	11.344	1.00	8.29
ATOM	1016	N	ASN	127	23.951	27.081	9.554	1.00	
ATOM	1017	CA	ASN	127	22.618	26.839	10.081		6.96
ATOM	1018	CB	ASN	127	21.832			1.00	6.87
	1010	-2	2011	141	21.032	25.948	9.120	1.00	6.56

ATOM 1019 CG ASN 127 22.515 26.650 7.801 1.00 0.11 ATOM 1020 MD ASP 127 21.150 25.859 6.758 1.00 7.39 ATOM 1021 MD ASP 127 21.150 25.859 6.758 1.00 7.39 ATOM 1022 C ASN 127 21.150 25.859 6.758 1.00 7.39 ATOM 1022 K ASN 127 23.503 25.153 11.763 1.00 7.00 ATOM 1023 K AVAL 128 21.2964 25.811 12.301 1.00 8.70 ATOM 1025 CA VAL 128 21.296 25.811 12.301 1.00 8.70 ATOM 1026 CB VAL 128 21.296 25.811 12.301 1.00 8.70 ATOM 1027 CO1 VAL 128 21.296 25.811 12.301 1.00 8.70 ATOM 1027 CO1 VAL 128 21.296 25.801 12.301 1.00 8.70 ATOM 1028 CC VAL 128 21.296 25.801 12.301 1.00 8.70 ATOM 1027 CO1 VAL 128 21.90 6.75 8.74 ATOM 1027 CO1 VAL 128 21.90 6.70 8.70 ATOM 1020 C VAL 128 19.906 27.774 14.501 1.00 9.46 ATOM 1021 C A TRP 129 19.907 23.102 25.032 13.239 1.00 7.79 ATOM 1031 C A TRP 129 19.907 23.103 13.62 13.60 7.79 ATOM 1031 C A TRP 129 18.834 22.103 13.62 1.00 7.79 ATOM 1031 C A TRP 129 19.804 22.103 13.62 1.00 7.98 ATOM 1031 C A TRP 129 19.804 22.103 13.62 1.00 7.99 ATOM 1034 CC TRP 139 19.46 22.215 11.53 1.00 7.47 ATOM 1035 CD TRP 139 17.353 22.488 10.400 1.00 6.77 ATOM 1036 CD TRP 139 17.353 22.488 10.400 1.00 6.77 ATOM 1037 C B TRP 129 19.466 22.215 11.53 1.00 6.79 ATOM 1037 C B TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1038 CD TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1039 C B TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1031 C B TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1034 C C B TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1035 CD TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1036 CD TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1037 C B TRP 129 19.466 22.215 11.50 1.00 6.79 ATOM 1044 C C B TRP 139 17.353 22.428 10.400 11.00 6.79 ATOM 1051 C B TRP 129 19.466 22.215 11.50 1.00 6.60 6.21 ATOM 1052 C B TRP 129 19.466 22.215 11.50 1.00 6.60 6.21 ATOM 1053 C B TRP 129 19.466 22.215 11.50 1.00 6.60 6.21 ATOM 1054 C B TRP 139 17.353 22.428 11.00 9.30 6.60 6.22 ATOM 1055 C B TRP 139 17.353 22.438 10.400 11.00 6.77 ATOM 1054 C B TRP 139 19.466 22.215 11.00 6.60 77 ATOM 1056 C B TRP 130 10.00 6.77 11.00 6.60 77 ATOM 1056 C B TRP 130 10.						- 93 -				
ATOM 1019 CS ASN 127 11.150 27.877 7.793 1.00 7.12 ATOM 1021 DD1 ASN 127 11.150 25.859 6.758 1.00 7.21 ATOM 1021 CD ASN 127 32.634 26.173 11.447 1.00 7.21 ATOM 1021 CD ASN 127 32.634 26.173 11.447 1.00 7.05 ATOM 1023 C ASN 127 32.634 26.173 11.447 1.00 7.05 ATOM 1023 C ASN 127 32.634 26.173 11.447 1.00 7.06 ATOM 1025 CA VAL 128 21.596 26.511 12.239 1.00 7.06 ATOM 1026 CE VAL 128 21.596 26.511 12.239 1.00 10.63 ATOM 1027 CG1 VAL 128 21.596 27.777 44 14.825 1.00 10.63 ATOM 1028 C C2 VAL 138 12.992 27.077 77 44 14.825 1.00 10.63 ATOM 1029 C C2 VAL 138 12.992 27.078 11.329 1.00 6.59 ATOM 1030 C C C VAL 128 12.91 10.01 ATOM 1031 C C C TRP 129 19.101 10.101 ATOM 1031 C C C TRP 129 19.101 10.101 ATOM 1032 C C TRP 129 19.501 10.101 ATOM 1033 C C TRP 129 19.501 10.101 ATOM 1034 C C TRP 129 19.501 10.60 11.601 ATOM 1035 C C TRP 129 18.844 22.914 13.851 1.00 7.799 ATOM 1036 C C TRP 129 19.501 10.60 11.001 ATOM 1036 C C TRP 129 19.501 10.60 11.001 ATOM 1037 C C TRP 129 19.501 10.60						515	26 650	7.803	1.00	6.11
ATOM 1021 ND2 ASM 1.7 21.150 25.559 6.758 1.00 7.23 ATOM 1021 ND2 C SS 1127 22.624 25.473 11.447 1.00 7.23 ATOM 1022 C SS 1127 22.624 25.473 11.447 1.00 7.06 ATOM 1023 C SS 1127 22.624 25.431 11.447 1.00 7.06 ATOM 1023 C SS 127 22.624 25.431 11.763 1.10 7.06 ATOM 1024 C SS 12.122 25.96 11.10 1.00 7.06 ATOM 1025 C C VAL 128 21.596 25.513 12.00 1.00 8.77 ATOM 1027 CC1 VAL 128 21.524 25.438 11.50.1 1.00 9.46 ATOM 1028 CC2 VAL 138 22.596 27.774 14.501 1.00 9.46 ATOM 1029 C VAL 138 19.101 25.426 12.617 1.00 8.76 ATOM 1029 C VAL 138 19.101 25.426 12.617 1.00 6.59 ATOM 1029 C VAL 138 19.101 25.426 12.617 1.00 6.59 ATOM 1029 C VAL 138 19.977 23.661 11.323 1.00 7.79 ATOM 1021 C R TRP 129 18.844 22.914 13.822 1.00 7.79 ATOM 1021 C R TRP 129 18.844 22.914 13.822 1.00 7.79 ATOM 1022 C R TRP 129 18.844 22.914 13.822 1.00 7.79 ATOM 1031 C TRP 129 20.807 22.488 10.495 1.00 6.77 ATOM 1031 C TRP 129 20.807 22.488 10.495 1.00 6.77 ATOM 1034 C TRP 129 20.807 22.488 10.495 1.00 6.77 ATOM 1035 C TRP 129 1.755 22.488 10.400 1.00 6.42 ATOM 1036 C TRP 129 1.755 22.488 10.400 1.00 6.42 ATOM 1037 C TRP 129 1.89 1.89 1.89 1.00 1.00 6.43 ATOM 1038 C TRP 129 1.755 22.488 10.400 1.00 6.43 ATOM 1039 C TRP 129 1.755 22.489 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 22.489 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 22.489 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 22.489 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 22.195 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 22.195 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 22.195 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 22.195 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.757 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.757 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.757 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.757 1.00 1.00 1.00 6.43 ATOM 1040 C TRP 129 1.755 1.755 1.757 1.00 1.00 1.00 6.43 AT	ATOM	1019							1.00	
ATOM 1022 C ASN 137 22.054 25.173 11.447 1.00 7.20 8.45 ATOM 1022 C ASN 137 22.054 25.153 11.763 1.00 8.46 ATOM 1023 C ASN 137 23.953 25.553 11.763 1.00 8.46 ATOM 1024 C ASN 137 23.953 25.553 11.763 1.00 8.46 ATOM 1024 C B VAL 128 21.254 25.459 13.501 1.00 10.65 ATOM 1027 C B VAL 128 21.254 25.459 13.501 1.00 10.65 ATOM 1027 C B VAL 128 21.254 25.459 13.501 1.00 10.65 ATOM 1029 C VAL 128 21.00 12.502 ATOM 1029 C VAL 128 20.032 25.003 27.501 11.002 10.65 ATOM 1029 C VAL 128 20.032 25.003 27.501 11.002 10.65 ATOM 1030 C VAL 128 20.032 25.003 27.501 11.002 10.65 ATOM 1030 C VAL 128 20.032 25.003 27.501 11.002 10.65 ATOM 1031 N TAPP 129 13.516 21.709 12.501 10.00 7.785 ATOM 1030 C TAPP 129 13.516 21.709 12.501 10.00 7.785 ATOM 1031 N TAPP 129 13.516 21.709 12.501 10.00 7.785 ATOM 1032 C TAPP 129 13.516 21.709 12.2555 1.00 7.785 ATOM 1033 C TAPP 129 13.516 21.709 12.2555 1.00 7.785 ATOM 1034 C TAPP 129 13.516 21.709 12.2555 1.00 7.785 ATOM 1035 C TAPP 129 13.516 21.709 12.2555 1.00 7.785 ATOM 1035 C TAPP 129 13.516 21.709 12.2555 1.00 6.77 ATOM 1036 C TAPP 129 13.516 21.709 12.2555 1.00 6.77 ATOM 1036 C TAPP 129 13.516 21.709 12.2555 1.00 6.77 ATOM 1036 C TAPP 129 13.516 21.709 12.2555 1.00 6.77 ATOM 1036 C TAPP 129 13.516 21.709 12.2555 1.00 6.77 ATOM 1036 C TAPP 129 13.500 ATOM 1037 C TAPP 129 13.500 ATOM 1036 C TAPP 129 13.500 ATOM 1037 C TAPP 129 13.500 ATOM 1036 C TAPP 129 13.500		1020						6.758	1.00	
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ATON: 1039 C		1028								
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ATOM 1036 CB2 TRD 129 19.486 22.838 9.368 1.00 6.42 ATOM 1037 CB3 TRD 129 17.552 22.438 10.400 1.00 6.42 ATOM 1037 CB3 TRD 129 12.9 17.552 22.438 11.031 1.00 6.42 ATOM 1039 CD1 TRD 129 20.887 22.349 11.031 1.00 8.83 ATOM 1040 CZ2 TRD 129 20.887 22.349 11.031 1.00 8.83 ATOM 1040 CZ2 TRD 129 129.909 22.765 9.771 1.00 8.83 ATOM 1041 CZ3 TRD 129 12.909 22.31.96 8.160 1.00 6.83 ATOM 1041 CZ3 TRD 129 12.916.754 22.796 9.207 1.00 7.42 ATOM 1041 CZ3 TRD 129 12.7553 23.187 8.120 1.00 6.83 ATOM 1042 CT TRD 129 18.902 23.196 8.160 1.00 6.83 ATOM 1043 C TRD 129 18.434 22.394 15.187 1.00 8.16 ATOM 1043 C TRD 129 18.7553 23.187 8.120 1.00 8.16 ATOM 1044 C TRD 130 17.158 22.208 15.321 1.00 9.10 ATOM 1046 C TRD 130 16.078 22.208 15.321 1.00 9.10 ATOM 1047 CA PBO 130 16.078 22.208 14.338 1.00 11.04 ATOM 1047 CA PBO 130 16.078 22.208 14.338 1.00 11.04 ATOM 1048 C FBO 130 18.87 21.348 14.930 1.00 12.74 ATOM 1049 CG PBO 130 18.97 21.348 14.930 1.00 12.79 ATOM 1050 C PBO 130 17.995 20.019 16.674 1.00 10.76 ATOM 1051 O PBO 130 17.992 20.019 16.674 1.00 10.76 ATOM 1051 O PBO 130 17.992 19.747 15.742 1.00 10.76 ATOM 1053 CA ASP 131 17.339 19.412 17.840 1.00 12.19 ATOM 1055 CC ASP 131 17.339 19.412 17.840 1.00 12.79 ATOM 1055 CC ASP 131 18.20 13.00 19.75 20.122 1.00 14.57 ATOM 1055 CC ASP 131 18.20 13.07 20.474 1.00 10.75 ATOM 1055 CC ASP 131 18.20 13.07 20.474 1.00 10.75 ATOM 1056 CB ASP 131 19.218 19.075 20.122 1.00 14.57 ATOM 1056 CB ASP 131 19.218 19.075 20.122 1.00 14.57 ATOM 1056 CB ASP 131 19.218 19.075 20.122 1.00 14.57 ATOM 1056 CB ASP 131 19.218 19.075 20.122 1.00 14.59 ATOM 1056 CB ASP 131 18.10 13.17.01 11.00 13.05 ATOM 1056 CB ASP 131 18.10 13.17.331 17.695 19.499 1.00 13.05 ATOM 1056 CB ASP 131 18.10 13.17.40 11.30 13.05 ATOM 1056 CB ASP 131 18.10 13.10 14.10 14.10 14.30 1.00 13.35 ATOM 1056 CB ASP 131 18.10 14.41 14.16 14.986 1.00 14.50 ATOM 1067 CB ASP 131 18.10 19.218 19.075 20.122 1.00 14.50 ATOM 1068 CB ASP 131 18.10 19.05 18.566 1.00 13.05 ATOM 1069 N THE 133 15.20 11.30 13.50 13.50 13.50 ATOM 1068 CB ASP 131 18.20	MOTA									
ATOM 1037 CE2 TRP 129 17.353 22.428 10.400 1.00 8.43 ATOM 1033 CD1 TRP 129 20.809 22.756 9.721 1.00 8.43 ATOM 1039 ME1 TRP 129 20.809 22.756 9.721 1.00 8.43 ATOM 1040 CZ2 TRP 129 129.809 22.756 9.721 1.00 6.63 ATOM 1040 CZ2 TRP 129 18.902 23.196 8.120 1.00 6.63 ATOM 1041 CZ1 TRP 129 18.902 23.196 8.120 1.00 6.84 ATOM 1042 CH2 TRP 129 18.434 22.394 15.187 1.00 6.84 ATOM 1042 CH2 TRP 129 18.434 22.394 15.187 1.00 8.13 ATOM 1044 O TRP 129 17.551 23.187 8.120 1.00 6.84 ATOM 1044 O TRP 129 17.551 23.187 8.120 1.00 9.20 ATOM 1045 N PRO 130 17.158 22.038 15.321 1.00 9.10 ATOM 1046 CD PRO 130 17.158 22.038 15.321 1.00 9.10 ATOM 1047 C PRO 130 16.684 21.410 16.563 1.00 11.04 ATOM 1047 C PRO 130 16.684 21.410 16.563 1.00 11.04 ATOM 1048 CB PRO 130 16.987 21.348 14.930 1.00 12.74 ATOM 1048 CB PRO 130 17.925 20.019 16.674 1.00 12.74 ATOM 1050 C PRO 130 17.925 20.019 16.674 1.00 10.75 ATOM 1051 O PRO 130 17.925 20.019 16.674 1.00 10.75 ATOM 1052 N ASP 131 17.311 17.651 18.063 18.062 1.00 10.75 ATOM 1053 CA ASP 131 17.311 17.651 18.063 18.062 1.00 12.38 ATOM 1053 CA ASP 131 17.311 17.651 18.063 18.062 1.00 12.38 ATOM 1053 CA ASP 131 17.311 17.691 19.099 1.00 20.75 ATOM 1055 CO ASP 131 17.311 17.691 19.099 1.00 20.75 ATOM 1055 C ASP 131 17.311 17.691 19.099 1.00 20.75 ATOM 1055 C ASP 131 18.290 18.307 20.474 1.00 10.75 ATOM 1055 C ASP 131 16.864 17.707 17.175 1.00 12.219 ATOM 1055 C ASP 131 16.864 17.707 17.175 1.00 12.22 ATOM 1055 C ASP 131 16.864 17.707 17.175 1.00 12.22 ATOM 1055 C ASP 131 16.864 17.707 17.175 1.00 12.22 ATOM 1056 C ASP 131 16.864 17.707 17.175 1.00 12.23 ATOM 1056 C ASP 131 16.864 17.7091 17.104 1.00 11.37 ATOM 1056 C ASP 131 18.104 17.991 17.104 1.00 11.37 ATOM 1056 C ASP 131 18.104 17.991 17.104 1.00 11.37 ATOM 1056 C ASP 131 18.104 17.991 17.104 1.00 11.37 ATOM 1056 C ASP 131 18.104 17.991 17.104 1.00 11.37 ATOM 1056 C ASP 131 18.104 17.991 17.104 1.00 11.37 ATOM 1056 C ASP 131 18.104 17.991 17.104 1.00 11.37 ATOM 1056 C ASP 131 18.90 18.90 18.90 18.90 18.90 18.90 18.90 18.90 18.90 18.90 18.90 18.90 18	ATOM							9.368		
ATOM 1038 CD1 TRP 129 20.887 22.349 11.031 A.00 8.43 ATOM 1039 MB1 TRP 129 20.887 22.349 11.031 A.00 8.43 ATOM 1040 CZ2 TRP 129 129.890 22.765 9.721 1.00 8.43 ATOM 1040 CZ2 TRP 129 12.990 23.196 8.160 1.00 7.42 ATOM 1041 CZ3 TRP 129 16.754 22.796 9.207 1.00 7.42 ATOM 1041 CZ3 TRP 129 16.754 22.796 9.207 1.00 7.42 ATOM 1043 C TRP 129 16.754 22.196 16.108 1.00 9.20 ATOM 1043 C TRP 129 18.902 23.187 15.187 1.00 8.10 ATOM 1043 C TRP 129 18.902 23.187 15.187 1.00 8.10 ATOM 1045 H PRO 130 17.158 22.208 15.321 1.00 9.20 ATOM 1045 H PRO 130 16.078 22.208 15.321 1.00 9.20 ATOM 1046 CD PRO 130 16.078 22.208 15.321 1.00 9.20 ATOM 1047 CA PRO 130 16.078 22.208 14.338 1.00 12.74 ATOM 1047 CA PRO 130 16.684 21.440 16.553 1.00 12.74 ATOM 1049 CG PRO 130 18.897 21.348 14.930 1.00 12.79 ATOM 1049 CG PRO 130 18.987 21.348 14.930 1.00 12.79 ATOM 1050 C PRO 130 17.925 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.925 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.925 20.019 16.674 1.00 10.76 ATOM 1052 N ASP 131 17.139 19.412 17.840 1.00 12.19 ATOM 1053 CA ASP 131 17.139 19.412 17.840 1.00 12.19 ATOM 1053 CA ASP 131 17.131 17.092 19.473 15.742 1.00 10.41 ATOM 1055 CG ASP 131 17.131 17.092 19.479 17.840 1.00 12.74 ATOM 1055 CG ASP 131 18.200 18.307 20.474 1.00 30.05 ATOM 1055 CG ASP 131 18.200 18.307 20.474 1.00 10.75 ATOM 1055 CG ASP 131 18.200 18.307 20.474 1.00 10.75 ATOM 1055 CG ASP 131 18.10 17.131 17.091 17.794 22.678 1.00 44.79 ATOM 1056 CB ASP 131 17.004 13.00 13.05 ATOM 1056 CB ASP 131 18.10 17.004 13.05 ATOM 1056 CB ASP 131 17.004 13.00 13.05 ATOM 1056 CB ASP 131 18.10 17.004 13.617 17.004 13.00 13.05 ATOM 1056 CB ASP 131 18.100 13.100 13.100 13.05 ATOM 1056 CB ASP 131 18.100 13.100 13.100 13.05 ATOM 1056 CB ASP 131 18.100 13.100 13.05 ATOM 1056 CB ASP 131 18.100 13.100 13.100 13.05 ATOM 1056 CB ASP 131 18.100 13.100 13.100 13.05 ATOM 1056 CB ASP 131 18.100 13.100 13.05 ATOM 1056 CB ASP 131 18.100 13.100 13.100 13.05 ATOM 1056 CB ASP 131 13.100 13.100 13.100 13.05 ATOM 1056 CB ASP 131 13.100 13.100 13.05 ATOM 1056 CB AS	MOTA						22.428	10.400		
ATOM 1038 CUI RRP 129 20.809 22.765 9.721 1.00 6.83 ATOM 1040 CZ2 TRP 129 18.902 33.196 8.160 1.00 6.83 ATOM 1041 CZ3 TRP 129 18.902 33.196 8.160 1.00 6.83 ATOM 1041 CZ3 TRP 129 18.7551 23.187 8.120 1.00 6.84 ATOM 1042 CH2 TRP 129 18.434 22.394 15.187 1.00 8.10 ATOM 1043 C TRP 129 18.434 22.394 15.187 1.00 8.10 ATOM 1044 O TRP 129 17.551 23.187 8.120 1.00 9.20 ATOM 1044 O TRP 129 17.552 23.187 8.120 1.00 9.20 ATOM 1045 N PRO 130 17.158 22.038 15.321 1.00 9.10 ATOM 1046 CD PRO 130 16.684 21.410 16.563 1.00 11.04 ATOM 1047 CA PRO 130 16.684 21.410 16.563 1.00 10.04 ATOM 1048 CB PRO 130 16.897 21.348 14.930 1.00 12.74 ATOM 1049 CG PRO 130 17.195 20.019 16.674 1.00 10.75 ATOM 1050 C PRO 130 17.992 19.473 ATOM 1051 O PRO 130 17.195 20.019 16.674 1.00 10.76 ATOM 1052 N ASP 131 17.139 19.471 15.742 1.00 10.41 ATOM 1052 N ASP 131 17.611 18.063 18.062 1.00 12.19 ATOM 1053 CA ASP 131 17.611 18.063 18.062 1.00 12.38 ATOM 1054 CB ASP 131 17.611 18.063 18.062 1.00 13.83 ATOM 1055 CO ASP 131 17.911 17.695 19.479 1.00 20.75 ATOM 1055 CO ASP 131 17.911 17.695 19.479 1.00 20.75 ATOM 1055 CO ASP 131 17.911 17.695 19.499 1.00 20.75 ATOM 1055 CO ASP 131 17.911 17.695 19.499 1.00 20.75 ATOM 1056 ODI ASP 131 19.218 19.075 20.122 1.00 14.54 ATOM 1056 CO ASP 131 17.912 19.13 19.75 20.012 12.219 ATOM 1056 CO ASP 131 17.912 19.13 19.75 20.012 19.10 19.715 19.715 19.00 12.219 ATOM 1056 CO ASP 131 16.684 17.091 17.104 1.00 13.38 ATOM 1056 CO ASP 131 17.912 19.473 17.104 1.00 12.219 ATOM 1057 CG ASP 131 18.11 17.924 19.091 17.104 1.00 13.37 ATOM 1058 C ASP 131 17.912 19.483 19.75 19.10 17.104 1.00 13.37 ATOM 1050 C B GUU 132 17.522 16.204 16.561 1.00 13.37 ATOM 1056 CO ASP 131 18.11 17.922 19.93 1.00 14.20 ATOM 1057 CG LW 132 17.522 16.204 16.561 1.00 13.37 ATOM 1058 C ASP 131 16.643 17.929 19.75 10.00 13.96 ATOM 1057 CG LW 132 17.522 16.222 17.556 1.00 13.05 ATOM 1058 C ASP 131 15.193 19.205 19.555 10.00 14.00 ATOM 1058 C C HR 133 15.937 19.05 19.505 19.655 19.001 19.00 19.00 ATOM 1066 OEI GUU 132 17.522 11.00 19.663 19.00 19.00 19.00 ATO	ATOM						22.349			
ATOM 1049 C22 TRP 129 18,902 23,396 8.160 1.00 7.42 ATOM 1041 C23 TRP 129 18,002 23,396 8.160 1.00 7.42 ATOM 1041 C23 TRP 129 18,453 22,796 9.207 1.00 7.42 ATOM 1041 C23 TRP 129 17,553 23,187 8.120 1.00 8.10 ATOM 1043 C TRP 129 18,434 22,394 15,187 1.00 8.10 ATOM 1043 C TRP 129 18,434 22,394 15,187 1.00 9.20 ATOM 1045 N PRO 130 17,158 22,268 16,108 1.00 9.20 ATOM 1045 N PRO 130 16,007 22,288 16,108 1.00 10.04 ATOM 1045 N PRO 130 16,007 22,288 16,108 1.00 11.04 ATOM 1045 CD PRO 130 16,007 22,288 14,338 1.00 11.04 ATOM 1047 CA PRO 130 16,007 21,400 11.04 ATOM 1049 CB PRO 130 15,190 21,366 16,377 1.00 12,74 ATOM 1049 CG PRO 130 15,190 21,366 16,377 1.00 12,74 ATOM 1050 C PRO 130 17,295 20,019 16,674 1.00 10,76 ATOM 1051 O PRO 130 17,902 19,473 15,742 1.00 10,41 ATOM 1051 O PRO 130 17,902 19,473 15,742 1.00 10,41 ATOM 1052 C RASP 131 17,611 18,063 18,062 1.00 13,83 ATOM 1053 CB ASP 131 17,611 18,063 18,062 1.00 13,83 ATOM 1055 CC ASP 131 17,611 18,063 18,062 1.00 13,83 ATOM 1055 CC ASP 131 19,181 17,611 18,063 18,062 1.00 10,76 ATOM 1055 CD ASP 131 19,288 19,075 20,122 1.00 41,54 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 41,54 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 41,54 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 41,54 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 41,54 ATOM 1056 OD1 ASP 131 18,111 17,7974 21,678 1.00 12,28 ATOM 1056 OD1 ASP 131 18,111 17,7974 21,678 1.00 12,28 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 44,79 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 11,37 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 11,37 ATOM 1056 OD1 ASP 131 19,288 19,075 20,122 1.00 11,37 ATOM 1060 OD1 ASP 131 19,288 19,075 20,122 1.00 11,37 ATOM 1060 OD1 ASP 131 19,288 19,075 20,122 1.00 11,37 ATOM 1060 OD1 ASP 131 19,288 19,075 20,122 1.00 11,37 ATOM 1060 OD1 ASP 131 19,288 19,075 20,122 1.00 11,37 ATOM 1060 OD1 ASP 131 19,288 19,075 20,122 19,00 14,30 14	ATOM									
ATOM 1040 C23 TRP 129 16.754 22.796 9.207 1.00 6.84 ATOM 1042 CH2 TRP 129 17.553 23.187 8.120 1.00 8.10 ATOM 1042 CH2 TRP 129 18.434 22.394 15.187 1.00 8.10 ATOM 1044 O TRP 129 18.434 22.394 15.187 1.00 9.20 ATOM 1044 O TRP 129 19.266 22.268 16.108 1.00 9.20 ATOM 1044 O TRP 129 19.266 22.268 16.108 1.00 9.20 ATOM 1045 N PRO 130 16.078 22.208 14.338 1.00 11.04 ATOM 1046 CD PRO 130 16.684 21.410 16.563 1.00 10.04 ATOM 1047 CA PRO 130 16.684 21.410 16.563 1.00 10.04 ATOM 1048 CB PRO 130 14.987 21.366 16.377 1.00 12.74 ATOM 1048 CG PRO 130 14.987 21.366 16.377 1.00 12.74 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.902 19.473 15.742 1.00 10.41 ATOM 1052 N ASP 131 17.339 19.412 17.840 1.00 12.19 ATOM 1052 N ASP 131 17.611 18.063 18.062 1.00 13.83 ATOM 1054 CB ASP 131 17.561 18.063 19.499 1.00 20.75 ATOM 1055 CC ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CC ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1056 ODL ASP 131 18.290 18.307 20.474 1.00 10.45 ATOM 1057 ODL ASP 131 18.11 17.974 21.678 1.00 44.79 ATOM 1056 ODL ASP 131 18.11 17.974 21.678 1.00 41.54 ATOM 1057 ODL ASP 131 18.11 17.974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.11 17.974 21.678 1.00 11.37 ATOM 1056 C ASP 131 18.10 11.7974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.10 11.7974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.10 11.7974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.11 17.974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.11 17.974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.11 17.974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.11 17.974 21.678 1.00 11.37 ATOM 1056 OL ASP 131 18.10 14.416 14.986 1.00 14.79 ATOM 1056 OL ASP 131 18.10 14.416 14.986 1.00 14.20 ATOM 1056 OL ASP 131 18.10 14.416 14.986 1.00 14.30 ATOM 1057 OL ASP 131 18.10 14.416 14.986 1.00 14.30 ATOM 1057 OL ASP 131 18.10 14.416 14.986 1.00 14.30 ATOM 1058 OL ASP 131 18.10 132 17.567 18.994 1.00 13.37 ATOM 1060 N GLU 132 17.667 13.50 14.410 19.40 11.30 1.00 13.36 ATOM 1060 OL ASP 131 18.30 18.30 19.30 19.3	A'TOM									
ATOM 1041 C43 TRF 129 17.553 23.187 8.120 1.00 8.30 ATOM 1043 C TRF 129 18.434 22.394 15.187 1.00 8.10 ATOM 1043 C TRF 129 19.266 22.268 16.108 1.00 9.20 ATOM 1045 N PRO 130 17.158 22.088 15.221 1.00 9.10 ATOM 1046 CD PRO 130 16.078 22.208 14.338 1.00 11.04 ATOM 1046 CD PRO 130 15.190 21.366 16.577 1.00 12.74 ATOM 1047 CA PRO 130 15.190 21.366 16.377 1.00 12.74 ATOM 1049 CB PRO 130 15.190 21.366 16.377 1.00 12.74 ATOM 1049 CG PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1055 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1055 C ASP 131 17.511 18.063 18.062 18.062 1.00 20.75 ATOM 1055 C ASP 131 17.511 18.063 18.062 18.062 1.00 20.75 ATOM 1055 C ASP 131 17.511 17.637 20.474 1.00 10.41 ATOM 1055 C ASP 131 17.511 17.597 20.474 1.00 10.45 ATOM 1056 C ASP 131 17.511 17.597 20.474 1.00 10.45 ATOM 1057 CD2 ASP 131 18.290 18.307 20.424 1.00 10.76 ATOM 1058 C ASP 131 17.511 17.577 20.1678 1.00 10.30.05 ATOM 1056 C ASP 131 17.511 17.577 20.1678 1.00 10.228 ATOM 1056 C ASP 131 18.211 17.577 1.175 1.00 10.41.37 ATOM 1056 C ASP 131 18.211 17.577 1.175 1.00 12.28 ATOM 1056 C ASP 131 18.211 17.577 1.175 1.00 12.28 ATOM 1056 C ASP 131 18.211 17.577 1.175 1.00 11.37 ATOM 1056 C ASP 131 18.211 17.577 17.175 1.00 12.28 ATOM 1056 N GLU 132 17.622 16.204 16.561 1.00 11.37 ATOM 1066 N GLU 132 17.622 16.204 16.561 1.00 11.37 ATOM 1066 N GLU 132 17.622 18.204 18.205 18.205 1.00 13.36 ATOM 1066 N GLU 132 17.004 13.217 14.169 1.00 11.37 ATOM 1066 N GLU 132 17.004 13.217 14.280 1.00 1.00 12.28 ATOM 1067 O C THR 133 15.291 13.055 18.297 1.00 14.30 ATOM 1068 N GLU 132 17.004 13.217 14.30 12.391 1.00 13.05 ATOM 1069 N GLU 132 17.004 13.567 12.395 1.00 14.30 ATOM 1066 N THR 133 15.291 13.005 18.591 1.00 13.05 ATOM 1067 N GLU 132 17.004 13.591 13.005 18.591 1.00 13.05 ATOM 1068 C C THR 133 15.911 12.663 19.645 1.00 13.05 ATOM 1068 C C THR 133 15.911 13.005 18.591 1.00 13.05 ATOM 1077 C C THR 133 15.911 13.005 18.591 1.00 13.00 13.05 ATOM 107	MOTA						22.796			
ATOM 1042 C TRP 129 18.434 22.394 15.187 1.00 9.20 ATOM 1044 O TRP 129 19.266 22.268 16.108 1.00 9.20 ATOM 1044 O TRP 129 19.266 22.268 16.108 1.00 9.20 ATOM 1045 N PRO 130 17.158 22.038 15.321 1.00 9.10 ATOM 1046 CD PRO 130 16.684 21.410 16.563 1.00 11.04 ATOM 1046 CD PRO 130 16.684 21.410 16.563 1.00 10.04 ATOM 1047 CA PRO 130 16.684 21.410 16.563 1.00 10.04 ATOM 1048 CB PRO 130 14.987 21.366 16.377 1.00 12.74 ATOM 1048 CG PRO 130 14.987 21.366 16.377 1.00 12.74 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.295 20.019 16.674 1.00 10.41 ATOM 1052 N ASP 131 17.339 19.412 17.840 1.00 12.19 ATOM 1052 N ASP 131 17.511 18.053 18.062 1.00 13.83 ATOM 1054 CB ASP 131 17.511 17.653 19.499 1.00 20.75 ATOM 1055 CC ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CC ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1057 ODD ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1057 ODD ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1057 ODD ASP 131 18.111 17.974 21.678 1.00 41.54 ATOM 1056 CD ASP 131 18.111 17.974 21.678 1.00 41.54 ATOM 1056 C ASP 131 18.111 17.974 21.678 1.00 12.28 ATOM 1056 C ASP 131 18.111 17.974 21.678 1.00 12.28 ATOM 1056 C ASP 131 18.111 17.974 21.678 1.00 12.28 ATOM 1056 C ASP 131 18.111 17.974 21.678 1.00 11.37 ATOM 1066 CB GLU 132 17.632 18.100 14.406 ATOM 1061 CA GLU 132 17.657 18.206 11.00 11.37 ATOM 1066 CB GLU 132 17.657 18.206 11.00 11.37 ATOM 1066 CB GLU 132 17.657 18.206 11.00 14.02 ATOM 1067 CB GLU 132 17.024 18.209 1.00 14.20 ATOM 1068 N THR 133 15.931 18.301 19.499 1.00 13.95 ATOM 1067 CB GLU 132 17.094 13.617 12.890 1.00 14.20 ATOM 1069 N THR 133 15.931 19.295 11.00 14.20 ATOM 1069 N THR 133 15.931 19.493 1.00 13.95 ATOM 1069 N THR 133 15.931 19.493 1.00 13.95 ATOM 1069 N THR 133 15.931 19.493 1.00 13.95 ATOM 1069 N THR 133 15.931 19.493 1.00 14.20 ATOM 1069 N THR 133 15.931 19.493 1.00 14.20 ATOM 1069 N THR 133 15.931 19.493 1.00 14.20 ATOM 1069 N THR 133 15.931 19.493 1.00 14.20 ATOM 1069 N THR 133 15.931 19.493 1.00 1	MOTA						23.187			
ATOM 1044 O TRP 129 19.266 22.268 16.108 1.00 9.10 ATOM 1045 N PRO 130 17.158 22.038 15.321 1.00 9.10 ATOM 1046 CD PRO 130 16.078 22.208 14.338 1.00 10.94 ATOM 1047 CA PRO 130 16.078 22.208 14.338 1.00 10.94 ATOM 1047 CA PRO 130 16.684 21.410 16.563 1.00 10.94 ATOM 1049 CG PRO 130 15.190 21.366 16.377 1.00 12.74 ATOM 1049 CG PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1051 N ASP 131 17.295 20.019 16.674 1.00 10.76 ATOM 1051 N ASP 131 17.397 19.412 17.840 1.00 12.19 ATOM 1052 N ASP 131 17.397 19.412 17.840 1.00 12.19 ATOM 1053 CA ASP 131 17.611 18.063 18.062 1.00 12.19 ATOM 1054 CB ASP 131 17.311 18.063 18.062 1.00 20.75 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 20.75 ATOM 1056 ODI ASP 131 18.111 17.974 21.678 1.00 41.54 ATOM 1057 OD2 ASP 131 18.111 17.974 21.678 1.00 41.37 ATOM 1058 C ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1059 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.652 16.204 15.660 1.00 12.37 ATOM 1060 N GLU 132 17.652 16.204 15.660 1.00 12.37 ATOM 1061 CA GLU 132 17.657 13.216 13.986 1.00 14.40 ATOM 1061 CA GLU 132 17.667 13.217 14.190 10.01 13.96 ATOM 1066 OE2 GLU 132 17.052 15.236 15.660 1.00 12.37 ATOM 1066 OE2 GLU 132 17.067 13.231 14.169 1.00 13.96 ATOM 1066 OE2 GLU 132 17.067 13.231 14.169 1.00 13.96 ATOM 1066 OE2 GLU 132 17.067 13.231 14.169 1.00 13.96 ATOM 1067 C G GLU 132 17.067 13.231 14.733 12.391 1.00 13.96 ATOM 1067 C G LU 132 17.067 13.231 14.733 12.391 1.00 13.96 ATOM 1067 C G LU 132 17.067 13.231 14.733 12.391 1.00 13.96 ATOM 1067 C G LU 132 17.667 13.231 14.733 12.391 1.00 13.96 ATOM 1067 C G LU 132 17.667 13.231 14.733 12.391 1.00 13.96 ATOM 1069 N THR 133 15.391 13.668 18.267 1.00 17.13 ATOM 1066 OE2 GLU 132 16.022 13.953 15.730 1.00 13.96 ATOM 1067 C G LU 132 17.667 13.231 14.733 13.91 1.00 13.96 ATOM 1071 CB THR 133 15.931 13.669 18.267 1.00 17.13 ATOM 1068 O CB LVS 134 13.992 17.576 1.00 15.02 1.00 14.60 ATOM 1070 CC HR 133 15.914 12.669 11.994 11.00 14.05 ATOM 1070 CC HR 133 17.904 11.992 11.995 1	MOTA						22.394	15.187		
ATOM 1045 N PRO 130 17.158 22.038 15.321 1.00 11.04 ATOM 1046 CD PRO 130 16.078 22.208 14.338 1.00 11.04 ATOM 1046 CD PRO 130 16.078 22.208 14.338 1.00 11.04 ATOM 1047 CA PRO 130 16.584 21.410 16.563 1.00 10.94 ATOM 1048 CB PRO 130 15.190 21.366 16.377 1.00 12.74 ATOM 1048 CB PRO 130 17.295 20.019 16.674 14.90 1.00 12.90 ATOM 1050 C PRO 130 17.295 20.019 16.674 14.00 10.76 ATOM 1050 C PRO 130 17.295 20.019 16.674 14.00 10.76 ATOM 1051 N ASP 131 17.902 19.473 15.742 1.00 10.41 ATOM 1051 N ASP 131 17.902 19.473 15.742 1.00 10.41 ATOM 1053 CA ASP 131 17.511 18.063 18.062 1.00 13.83 ATOM 1053 CB ASP 131 17.511 17.655 19.499 1.00 20.75 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1057 OD2 ASP 131 18.191 17.974 21.678 1.00 44.79 ATOM 1058 C ASP 131 18.290 13.301 17.375 10.00 12.28 ATOM 1059 ON ASP 131 18.684 17.077 17.175 1.00 12.28 ATOM 1050 N GU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1050 N GU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1060 N GU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1061 CA GU 132 17.632 15.336 15.660 1.00 12.37 ATOM 1061 CA GU 132 17.032 15.336 15.660 1.00 12.37 ATOM 1066 OE2 GU 132 16.222 12.70 14.416 ATOM 1066 OE2 GU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1066 OE2 GU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1066 OE2 GU 132 16.222 12.70 13.617 12.890 1.00 14.02 ATOM 1066 OE2 GU 132 16.222 12.70 13.521 14.169 1.00 13.96 ATOM 1066 OE2 GU 132 16.022 12.70 13.617 12.890 1.00 14.02 ATOM 1067 C C UT 132 15.032 18.40 19.91 10.00 13.96 ATOM 1066 OE2 GU 132 16.222 12.70 13.617 12.890 1.00 14.02 ATOM 1067 C C UT 132 15.032 19.683 1.00 14.71 ATOM 1068 O GU 132 17.091 13.692 17.576 1.00 13.96 ATOM 1067 C C UT 132 15.022 13.953 19.645 1.00 14.02 ATOM 1067 C C UT 132 16.222 12.70 13.951 1.00 13.96 ATOM 1068 O GU 132 15.022 13.952 17.576 1.00 13.05 ATOM 1068 O GU 132 15.022 13.953 19.645 1.00 14.02 ATOM 1069 N HIS 133 15.391 13.992 15.664 1.00 14.00 14.00 ATOM 1070 CA THR 133 15.911 19.603 11.914 19.407 1.00 13.05 ATOM 1070 CA THR 133 15.391	MOTA						22.268			
ATOM 1045 N PRO 130 16.078 22.208 14.318 1.00 10.04 ATOM 1047 CA PRO 130 16.684 21.410 16.563 1.00 10.04 ATOM 1048 CB PRO 130 15.190 21.366 16.377 1.00 12.274 ATOM 1049 CG PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.902 19.473 15.742 1.00 10.41 ATOM 1051 O PRO 130 17.902 19.473 17.840 1.00 12.19 ATOM 1053 CA ASP 131 17.631 18.063 18.062 1.00 13.83 ATOM 1053 CB ASP 131 17.611 18.063 18.062 1.00 13.83 ATOM 1054 CB ASP 131 17.511 18.063 18.062 1.00 13.83 ATOM 1055 CG ASP 131 18.201 18.307 20.474 1.00 30.05 ATOM 1056 OD1 ASP 131 18.111 17.974 21.678 1.00 41.54 ATOM 1057 OD2 ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1058 C ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1050 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.692 15.226 15.660 1.00 12.37 ATOM 1061 CA GLU 132 17.693 15.226 15.660 1.00 12.37 ATOM 1062 CB GLU 132 17.693 15.226 15.660 1.00 12.37 ATOM 1066 OC GLU 132 17.693 15.226 15.660 1.00 12.37 ATOM 1066 OC GLU 132 17.693 15.236 15.660 1.00 12.37 ATOM 1066 OC GLU 132 17.693 15.236 15.660 1.00 12.37 ATOM 1066 OC GLU 132 17.693 15.236 15.660 1.00 12.37 ATOM 1066 OC GLU 132 17.693 15.236 15.660 1.00 12.37 ATOM 1066 OC GLU 132 17.697 13.211 14.169 1.00 14.02 ATOM 1066 OC GLU 132 17.697 13.211 14.169 1.00 13.96 ATOM 1066 OC GLU 132 17.697 13.211 14.169 1.00 13.96 ATOM 1067 C C GLU 132 17.697 13.211 14.731 12.890 1.00 14.20 ATOM 1067 C C GLU 132 17.697 13.211 14.731 12.890 1.00 14.02 ATOM 1067 C C GLU 132 17.697 13.617 12.890 1.00 14.02 ATOM 1067 C C GLU 132 17.697 13.617 12.890 1.00 14.02 ATOM 1069 N THR 133 15.291 13.921 1.00 13.96 ATOM 1067 C C GLU 132 15.022 13.953 15.730 1.00 13.96 ATOM 1067 C C THR 133 15.911 12.663 18.267 1.00 13.05 ATOM 1069 N THR 133 15.911 12.663 18.267 1.00 17.13 ATOM 1069 N THR 133 15.911 13.962 11.914 19.407 1.00 21.80 ATOM 1070 CA THR 133 15.915 13.964 11.00 14.05 ATOM 1070 C C THR 133 17.900 11.918 19.905 11.00 14.05 ATOM 1070 C C THR 133 17	ATOM									
ATOM 1047 CA PRO 130 16.684 21.410 16.563 1.00 12.74 ATOM 1048 CB PRO 130 15.190 21.366 16.377 1.00 12.74 ATOM 1049 CG PRO 130 15.190 21.366 16.377 1.00 12.79 ATOM 1049 CG PRO 130 17.902 19.473 15.742 1.00 10.75 ATOM 1051 O PRO 130 17.902 19.473 15.742 1.00 10.76 ATOM 1051 O PRO 130 17.902 19.473 15.742 1.00 10.41 ATOM 1051 N ASP 131 17.511 18.063 18.062 1.00 12.19 ATOM 1053 CA ASP 131 17.511 18.063 18.062 1.00 12.19 ATOM 1054 CB ASP 131 17.511 17.695 19.499 1.00 20.75 ATOM 1054 CB ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CO ASP 131 18.291 19.278 19.499 1.00 20.75 ATOM 1056 OD1 ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1056 OD ASP 131 18.111 17.974 21.678 1.00 41.54 ATOM 1056 OD ASP 131 16.864 17.077 17.175 1.00 12.28 ATOM 1059 O ASP 131 16.864 17.077 17.175 1.00 12.28 ATOM 1060 N GLU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1060 C B GLU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1060 C CB GLU 132 17.657 13.221 14.169 1.00 14.02 ATOM 1060 C CB GLU 132 17.667 13.221 44.169 1.00 14.02 ATOM 1065 OEI GLU 132 17.407 13.617 12.880 1.00 14.02 ATOM 1066 OEE GLU 132 17.607 13.221 14.169 1.00 14.02 ATOM 1066 N GLU 132 17.607 13.221 14.169 1.00 14.02 ATOM 1066 N GLU 132 17.004 13.617 12.880 1.00 14.02 ATOM 1067 C GLU 132 17.004 13.617 12.880 1.00 14.02 ATOM 1066 N GLU 132 17.007 13.617 12.880 1.00 14.02 ATOM 1067 C GLU 132 16.222 12.787 12.395 1.00 13.96 ATOM 1067 C GLU 132 16.222 12.787 12.395 1.00 13.95 ATOM 1067 C GLU 132 16.223 13.953 15.730 1.00 13.95 ATOM 1067 C GLU 132 17.602 14.90 13.617 12.880 1.00 17.13 ATOM 1067 C GLU 132 17.602 14.90 13.617 12.880 1.00 14.02 ATOM 1069 N THR 133 15.202 13.953 15.730 1.00 13.95 ATOM 1067 C GLU 132 17.602 14.90 14.90 14.90 14.90 14.90 ATOM 1070 CA THR 133 15.202 13.953 15.730 1.00 13.96 ATOM 1070 CA THR 133 15.202 13.953 15.766 1.00 17.13 ATOM 1068 C GLU 132 17.667 13.291 14.100 12.90 17.91 ATOM 1070 CA THR 133 15.291 15.663 19.645 1.00 19.10 ATOM 1070 CA THR 133 15.291 15.663 19.645 1.00 19.10 ATOM 1070 CB THR 133 15.91 19.602 19.633 1.00 16.10 ATOM 1070 CA THR 133 15.	MOTA						22.208			
ATOM 1047 CB PRO 130 15.190 21.366 16.377 1.00 12.39 ATOM 1049 CB PRO 130 14.987 21.348 14.930 1.00 12.39 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.76 ATOM 1051 O PRO 130 17.295 20.019 15.674 1.00 10.41 ATOM 1051 O PRO 130 17.992 19.473 15.742 1.00 10.41 ATOM 1052 N ASP 131 17.319 19.412 17.840 1.00 12.19 ATOM 1053 CA ASP 131 17.319 19.412 17.840 1.00 12.19 ATOM 1054 CB ASP 131 17.311 17.651 18.063 18.062 1.00 13.83 ATOM 1055 CO ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CO ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CO ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 OD1 ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1057 OD2 ASP 131 18.111 17.974 21.678 1.00 14.54 ATOM 1058 C ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1059 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1050 C CB GLU 132 17.032 15.236 15.660 1.00 12.23 ATOM 1060 N GLU 132 17.032 15.236 15.660 1.00 12.37 ATOM 1061 CB GLU 132 17.032 15.236 15.660 1.00 12.37 ATOM 1066 CG GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1066 OE2 GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1066 OE2 GLU 132 17.024 14.733 12.391 1.00 13.96 ATOM 1066 OE2 GLU 132 17.327 14.733 12.391 1.00 13.96 ATOM 1066 OE2 GLU 132 17.024 13.793 12.391 1.00 13.96 ATOM 1066 OE2 GLU 132 17.027 13.221 14.169 1.00 14.02 ATOM 1067 C GLU 132 17.027 13.77 14.733 12.391 1.00 13.96 ATOM 1069 N THR 133 15.293 13.593 15.730 1.00 13.96 ATOM 1069 N THR 133 15.931 13.065 18.267 1.00 13.05 ATOM 1069 N THR 133 15.931 13.065 18.267 1.00 13.05 ATOM 1070 CA THR 133 15.931 13.065 18.267 1.00 17.33 ATOM 1070 CA THR 133 16.283 13.992 17.576 1.00 14.30 ATOM 1070 CA THR 133 15.931 13.065 18.267 1.00 14.31 ATOM 1070 CA THR 133 15.931 12.663 19.407 1.00 14.81 ATOM 1071 CB THR 133 16.284 13.992 19.407 19.407 1.00 14.81 ATOM 1070 CA THR 133 16.284 13.992 19.407 19.407 1.00 14.81 ATOM 1070 CA THR 133 16.284 13.992 19.655 18.681 1.00 19.10 ATOM 1071 CB THR 133 16.286 17.7891 19.407 1.00 14.05 ATOM 1078 CB LYS 134 13.992 15.665 18.681 1.00 14.71 ATOM 1080 CC LYS 134 13.992 15.665 18.681 1.00 19.47	ATOM						21.410			
ATOM 1049 CG PRO 130 14.987 21.348 14.930 1.00 10.76 ATOM 1050 C PRO 130 17.295 20.019 16.674 1.00 10.47 ATOM 1051 0 PRO 130 17.902 19.473 15.742 1.00 10.41 ATOM 1052 N ASP 131 17.319 19.417 17.840 1.00 12.19 ATOM 1053 CA ASP 131 17.611 18.063 18.062 1.00 13.83 ATOM 1054 CB ASP 131 17.511 18.063 18.062 1.00 13.83 ATOM 1055 CG ASP 131 17.311 17.695 19.499 1.00 20.75 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CG ASP 131 18.218 19.075 20.122 1.00 41.54 ATOM 1056 OD1 ASP 131 18.111 17.974 21.678 1.00 14.79 ATOM 1056 C ASP 131 16.864 17.077 17.175 1.00 12.28 ATOM 1056 C ASP 131 16.864 17.077 17.175 1.00 12.28 ATOM 1059 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.627 16.204 16.561 1.00 11.37 ATOM 1061 CA GLU 132 17.667 13.221 14.169 1.00 14.40 ATOM 1063 CG GLU 132 17.667 13.221 14.169 1.00 14.02 ATOM 1064 CD GLU 132 17.067 13.617 12.890 1.00 14.20 ATOM 1065 OEI GLU 132 17.04 13.617 12.890 1.00 14.20 ATOM 1066 OE GLU 132 17.327 14.733 12.391 1.00 13.96 ATOM 1066 OE GLU 132 17.04 13.617 12.890 1.00 14.70 ATOM 1066 OE GLU 132 17.327 14.733 12.391 1.00 13.96 ATOM 1066 OE GLU 132 17.327 14.733 12.391 1.00 13.96 ATOM 1067 C G GLU 132 16.222 12.787 12.395 1.00 14.71 ATOM 1068 O GLU 132 16.028 14.309 16.327 1.00 13.05 ATOM 1067 C GTHR 133 15.337 13.065 18.267 1.00 13.05 ATOM 1067 C THR 133 15.317 12.663 19.645 1.00 17.33 ATOM 1067 CA THR 133 15.337 13.065 18.267 1.00 13.05 ATOM 1070 CA THR 133 15.911 12.663 19.645 1.00 14.31 ATOM 1077 CR LYS 134 13.992 15.065 18.691 1.00 14.05 ATOM 1077 CR LYS 134 13.992 15.065 18.691 1.00 14.05 ATOM 1078 CB LYS 134 13.992 15.065 18.691 1.00 14.05 ATOM 1079 CG THR 133 15.276 15.065 18.691 1.00 12.50 ATOM 1079 CG THR 133 17.379 18.052 19.593 1.00 14.71 ATOM 1070 CA THR 133 17.379 18.052 19.593 10.00 13.05 ATOM 1070 CA THR 133 17.379 18.052 19.593 10.00 14.70 ATOM 1071 CB THR 133 17.200 11.914 19.407 1.00 13.05 ATOM 1073 CG2 THR 133 17.379 18.052 19.593 10.00 14.05 ATOM 1077 CA LYS 134 11.992 15.065 18.691 1.00 12.50 ATOM 1088 C LYS 134 13.992 15.065 18	MOTA						21.366			
ATOM 1050 C PRO 130 17.295 20.019 16.574 1.00 10.1 1 1.00 1 1.0	MOTA						21.348			
ATOM 1051 0 PRO 130 17.902 19.473 15.742 1.00 12.19 ATOM 1052 N ASP 131 17.139 19.412 17.840 1.00 12.19 ATOM 1053 CA ASP 131 17.139 19.416 17.695 19.499 1.00 20.75 ATOM 1054 CB ASP 131 17.511 18.063 19.499 1.00 20.75 ATOM 1055 CG ASP 131 18.201 18.307 20.474 1.00 30.05 ATOM 1055 OD1 ASP 131 19.218 19.075 20.122 1.00 41.54 ATOM 1056 OD1 ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1057 OD2 ASP 131 18.111 17.974 21.678 1.00 12.28 ATOM 1058 C ASP 131 15.684 17.077 17.175 1.00 12.28 ATOM 1059 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.032 15.236 15.660 1.00 12.37 ATOM 1061 CA GLU 132 17.667 13.221 14.169 1.00 14.40 ATOM 1062 CB GLU 132 17.667 13.221 14.169 1.00 14.02 ATOM 1063 CG GLU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1064 CD GLU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1065 OE1 GLU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1066 OE2 GLU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1066 OE2 GLU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1066 OE2 GLU 132 17.004 13.950 15.370 10.00 13.96 ATOM 1067 C GLU 132 17.004 13.951 15.370 1.00 13.96 ATOM 1068 O GLU 132 16.222 12.787 12.395 1.00 14.71 ATOM 1068 O GLU 132 16.028 14.309 16.327 1.00 13.95 ATOM 1069 N THR 133 15.022 13.953 15.730 1.00 14.71 ATOM 1069 N THR 133 15.911 12.663 19.665 1.00 17.13 ATOM 1067 CA THR 133 15.912 12.663 19.665 1.00 19.30 ATOM 1070 CA THR 133 15.937 12.695 15.00 17.13 ATOM 1070 CB THR 133 15.917 12.663 19.665 1.00 19.30 ATOM 1071 CB THR 133 15.917 12.663 19.665 1.00 19.30 ATOM 1073 CG2 THR 133 17.200 11.914 19.407 1.00 21.80 ATOM 1076 CB CLYS 134 13.992 15.055 18.691 1.00 14.08 ATOM 1077 CA LYS 134 13.992 15.056 18.267 1.00 17.13 ATOM 1076 CB CB CLYS 134 13.992 15.056 18.267 1.00 14.08 ATOM 1077 CA LYS 134 13.992 15.056 18.267 1.00 17.13 ATOM 1079 CG CHYS 134 13.992 15.056 18.267 1.00 17.13 ATOM 1079 CG LYS 134 13.992 15.056 18.267 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.056 18.267 1.00 14.08 ATOM 1070 CG HRS 133 13.992 15.055 18.599 1.00 14.09 ATOM 1080 CD LYS 134 13.992 15.068 17.697 1.00 12.75	MOTA						20.019			
ATOM 1052 N ASP 131 17.139 19.412 17.840 1.00 13.83 ATOM 1053 CA ASP 131 17.131 17.651 18.062 1.00 13.83 ATOM 1054 CB ASP 131 17.311 17.655 19.499 1.00 20.75 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1056 OD1 ASP 131 18.291 19.075 20.122 1.00 41.54 ATOM 1057 OD2 ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1058 C ASP 131 18.111 17.974 21.678 1.00 12.28 ATOM 1059 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1061 CA GLU 132 17.632 15.236 15.660 1.00 12.37 ATOM 1062 CB GLU 132 17.667 13.221 14.169 1.00 14.40 ATOM 1063 CG GLU 132 17.067 13.221 14.169 1.00 14.20 ATOM 1064 CD GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1065 OE1 GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1066 OE2 GLU 132 15.202 12.787 12.395 1.00 14.71 ATOM 1066 OE2 GLU 132 15.022 12.787 12.395 1.00 13.96 ATOM 1067 C GLU 132 15.022 13.953 15.730 1.00 13.05 ATOM 1068 O GLU 132 15.022 13.953 15.730 1.00 13.05 ATOM 1069 N THR 133 16.283 13.922 17.576 1.00 13.05 ATOM 1069 N THR 133 16.283 13.922 17.576 1.00 13.05 ATOM 1069 N THR 133 16.283 13.922 17.576 1.00 15.02 ATOM 1070 CA THR 133 15.917 12.663 19.645 1.00 19.10 ATOM 1071 CB THR 133 15.917 12.663 19.645 1.00 19.10 ATOM 1073 CC2 THR 133 17.200 11.914 19.407 1.00 21.80 ATOM 1074 C THR 133 15.917 12.663 19.645 1.00 19.10 ATOM 1075 N LYS 134 13.992 15.055 18.681 1.00 14.81 ATOM 1076 C THR 133 15.917 12.663 19.645 1.00 14.81 ATOM 1077 CA LYS 134 13.992 15.055 18.681 1.00 14.81 ATOM 1079 CG LYS 134 13.092 17.851 18.943 1.00 14.81 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.83 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1088 CG HIS 135 11.890 17.498 23.	MOTA						19.473			
ATOM 1053 CA ASP 131 17.511 18.063 18.062 1.00 20.75 ATOM 1054 CB ASP 131 17.311 17.695 19.499 1.00 20.75 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1056 OD1 ASP 131 19.218 19.075 20.122 1.00 41.54 ATOM 1057 OD2 ASP 131 18.111 17.974 21.678 1.00 44.79 ATOM 1058 C ASP 131 18.111 17.974 21.678 1.00 12.28 ATOM 1058 C ASP 131 16.864 17.077 17.175 1.00 12.28 ATOM 1059 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.632 16.204 16.561 1.00 12.37 ATOM 1060 N GLU 132 17.032 15.236 15.660 1.00 12.37 ATOM 1061 CA GLU 132 17.032 15.236 15.660 1.00 12.37 ATOM 1063 CG GLU 132 18.140 14.416 14.986 1.00 14.40 ATOM 1063 CG GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1066 OE2 GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1066 OE2 GLU 132 16.222 12.787 12.395 1.00 14.71 ATOM 1066 OE2 GLU 132 16.222 12.787 12.395 1.00 14.71 ATOM 1068 O GLU 132 15.022 13.953 15.730 1.00 13.05 ATOM 1068 O GLU 132 15.022 13.953 15.730 1.00 13.05 ATOM 1069 N THR 133 15.397 13.065 18.267 1.00 13.01 ATOM 1070 CA THR 133 15.397 13.065 18.267 1.00 17.13 ATOM 1071 CB THR 133 15.21 13.817 20.436 1.00 17.13 ATOM 1072 CGI THR 133 15.21 13.817 20.436 1.00 13.81 ATOM 1075 O THR 133 15.911 12.663 19.645 1.00 19.10 ATOM 1070 CA THR 133 15.911 12.663 19.645 1.00 19.10 ATOM 1071 CB THR 133 15.911 12.663 19.645 1.00 19.10 ATOM 1072 CGI THR 133 15.911 12.663 19.645 1.00 19.10 ATOM 1075 O THR 133 15.911 12.663 19.645 1.00 18.31 ATOM 1076 CB LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1077 CA LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1078 CB LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 13.05 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 12.75 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 13.42 ATOM 1080 CD LYS 134 13.992 17.072 19.683 1.00 12.75 ATOM 1080 CD LYS 134 13.992 15.664 17	ATOM						19.412			
ATOM 1054 CB ASP 131 17.311 17.695 19.499 1.00 30.05 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1055 CG ASP 131 18.290 18.307 20.474 1.00 30.05 ATOM 1056 OD1 ASP 131 19.218 19.075 20.122 1.00 41.54 ATOM 1057 OD2 ASP 131 18.211 17.974 21.678 1.00 44.79 ATOM 1058 C ASP 131 16.644 17.077 17.175 1.00 12.28 ATOM 1059 O ASP 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1061 CA GLU 132 17.632 16.204 16.561 1.00 12.37 ATOM 1062 CB GLU 132 17.632 16.204 16.561 1.00 12.37 ATOM 1064 CD GLU 132 17.607 14.4169 1.00 14.02 ATOM 1064 CD GLU 132 17.607 13.221 14.169 1.00 14.02 ATOM 1064 CD GLU 132 17.004 13.617 12.890 1.00 14.02 ATOM 1066 OE2 GLU 132 16.222 12.787 12.395 1.00 14.71 ATOM 1066 OE2 GLU 132 16.222 12.787 12.395 1.00 14.71 ATOM 1067 C GLU 132 16.222 12.787 12.395 1.00 13.05 ATOM 1068 O GLU 132 15.221 14.33 12.2391 1.00 13.05 ATOM 1069 N THR 133 16.283 13.922 17.576 1.00 13.05 ATOM 1069 N THR 133 15.337 13.065 18.267 1.00 13.05 ATOM 1070 CA THR 133 15.337 13.065 18.267 1.00 17.13 ATOM 1071 CB THR 133 15.911 12.663 19.645 1.00 17.13 ATOM 1072 OG1 THR 133 16.214 13.817 20.436 1.00 19.10 ATOM 1074 C THR 133 17.700 13.055 18.581 1.00 14.81 ATOM 1075 O THR 133 17.700 13.788 18.504 1.00 19.10 ATOM 1075 O THR 133 17.700 13.055 18.581 1.00 14.81 ATOM 1077 CA LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 17.851 23.411 1.00 29.07 ATOM 1084 O LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 10.34 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 10.34 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 10.34 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 10.34 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 10.34	MOTA									
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ATOM 1059 O ASF 131 15.643 17.091 17.104 1.00 11.37 ATOM 1060 N GLU 132 17.632 16.204 16.561 1.00 11.37 ATOM 1061 CA GLU 132 17.032 15.236 15.660 1.00 12.37 ATOM 1061 CA GLU 132 17.032 15.236 15.660 1.00 14.40 ATOM 1062 CB GLU 132 17.667 13.221 14.169 1.00 14.02 ATOM 1063 CG GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1064 CD GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1065 OE1 GLU 132 17.327 14.733 12.391 1.00 13.96 ATOM 1066 OE2 GLU 132 16.028 14.309 16.327 1.00 13.96 ATOM 1066 OE2 GLU 132 16.028 14.309 16.327 1.00 13.05 ATOM 1068 O GLU 132 15.022 13.953 15.730 1.00 13.05 ATOM 1068 N THR 133 16.283 13.922 17.576 1.00 15.02 ATOM 1069 N THR 133 16.283 13.922 17.576 1.00 17.13 ATOM 1070 CA THR 133 15.397 13.065 18.267 1.00 17.13 ATOM 1071 CB THR 133 15.911 12.663 19.645 1.00 19.10 ATOM 1072 OG1 THR 133 16.214 13.817 20.436 1.00 30.56 ATOM 1073 CG2 THR 133 17.200 11.914 19.407 1.00 21.80 ATOM 1074 C THR 133 15.91 12.663 19.645 1.00 14.81 ATOM 1075 N LYS 134 13.992 15.065 18.681 1.00 14.81 ATOM 1076 N LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1077 CA LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.028 17.072 19.683 1.00 14.05 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 24.72 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 29.07 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1079 CG LYS 134 13.992 15.065 18.681 1.00 29.07 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CG LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CG LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CG LYS 134 13.992 15.065 18.681 1.00 12.50 ATOM 1080 CG LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CG LYS 134 13.992 16.084 17.673 1.00 12.75 ATOM 1080 CG LYS 134 13.992 16.084 17.673 1.00 12.75 ATOM 1080 CG HIS 135 12.568 18.014 17.697 1.00 10.34 ATOM 1080 CG HIS 135 12.568 18.017 1	MOTA						17.077			
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ATOM 1061 CA GLU 132 17.032 15.236 15.860 1.00 14.40 ATOM 1062 CB GLU 132 17.667 13.221 14.169 1.00 14.02 ATOM 1063 CG GLU 132 17.667 13.221 14.169 1.00 14.02 ATOM 1064 CD GLU 132 17.004 13.617 12.890 1.00 14.20 ATOM 1065 OE1 GLU 132 17.327 14.733 12.391 1.00 13.96 ATOM 1066 OE2 GLU 132 16.222 12.787 12.395 1.00 14.71 ATOM 1066 OE2 GLU 132 16.028 14.309 16.327 1.00 13.05 ATOM 1067 C GLU 132 15.022 13.953 15.730 1.00 13.21 ATOM 1068 N THR 133 16.283 13.922 17.576 1.00 15.02 ATOM 1069 N THR 133 16.283 13.922 17.576 1.00 17.13 ATOM 1070 CA THR 133 15.337 13.065 18.267 1.00 17.13 ATOM 1071 CB THR 133 15.911 12.663 19.645 1.00 19.10 ATOM 1072 OG1 THR 133 15.911 12.663 19.465 1.00 30.56 ATOM 1073 CG2 THR 133 17.200 11.914 19.407 1.00 21.80 ATOM 1074 C THR 133 14.003 13.738 18.504 1.00 14.81 ATOM 1075 O THR 133 12.976 13.052 18.539 1.00 18.31 ATOM 1076 N LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1077 CA LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1078 CB LYS 134 13.08 17.70 19.683 1.00 14.05 ATOM 1079 CG LYS 134 13.566 16.783 21.105 1.00 14.05 ATOM 1079 CG LYS 134 13.566 16.783 21.105 1.00 14.05 ATOM 1080 CD LYS 134 13.566 16.783 21.105 1.00 21.50 ATOM 1080 CD LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1080 CD LYS 134 13.566 16.783 21.105 1.00 24.72 ATOM 1081 CE LYS 134 13.566 16.783 21.105 1.00 24.72 ATOM 1080 CD LYS 134 13.566 16.783 21.105 1.00 24.72 ATOM 1081 CE LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1083 C LYS 134 13.739 18.052 23.411 1.00 29.07 ATOM 1080 CD LYS 134 13.566 16.783 21.105 1.00 21.50 ATOM 1081 CE LYS 134 13.992 15.065 18.064 17.677 1.00 12.75 ATOM 1082 NZ LYS 134 13.992 15.065 18.062 17.00 10.74 ATOM 1083 C LYS 134 11.982 16.084 17.677 1.00 12.75 ATOM 1084 C LYS 134 13.992 15.666 17.697 1.00 12.75 ATOM 1085 N HIS 135 12.268 18.091 17.498 23.673 1.00 11.72 ATOM 1088 CG HIS 135 12.568 18.091 17.592 1.00 10.34 ATOM 1089 CD HIS 135 12.568 18.091 15.664 1.00 11.74 ATOM 1089 CD HIS 135 12.568 18.091 17.592 1.00 10.34	MOTA									
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ATOM 1072 OG1 THR 133 16.214 13.817 20.430 1.00 21.80 ATOM 1073 CG2 THR 133 17.200 11.914 19.407 1.00 14.81 ATOM 1074 C THR 133 14.003 13.738 18.504 1.00 14.81 ATOM 1075 O THR 133 12.976 13.052 18.539 1.00 18.31 ATOM 1076 N LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1077 CA LYS 134 12.738 15.763 18.943 1.00 16.10 ATOM 1078 CB LYS 134 13.028 17.072 19.683 1.00 16.10 ATOM 1079 CG LYS 134 13.566 16.783 21.105 1.00 21.50 ATOM 1079 CG LYS 134 13.739 18.052 21.912 1.00 24.72 ATOM 1080 CD LYS 134 13.739 18.052 21.912 1.00 24.72 ATOM 1081 CE LYS 134 13.962 17.851 23.411 1.00 29.07 ATOM 1081 CE LYS 134 13.962 17.851 23.411 1.00 29.07 ATOM 1082 NZ LYS 134 15.380 17.498 23.673 1.00 35.66 ATOM 1083 C LYS 134 15.380 17.498 23.673 1.00 35.66 ATOM 1083 C LYS 134 10.764 16.268 17.697 1.00 11.72 ATOM 1084 O LYS 134 10.764 16.268 17.697 1.00 12.75 ATOM 1085 N HIS 135 12.768 16.210 16.602 1.00 10.34 ATOM 1085 CA HIS 135 12.229 16.559 15.278 1.00 9.70 ATOM 1086 CA HIS 135 12.229 16.559 15.278 1.00 10.46 ATOM 1087 CB HIS 135 12.568 18.014 14.927 1.00 10.46 ATOM 1088 CG HIS 135 11.859 18.971 15.855 1.00 11.74 ATOM 1089 CD2 HIS 135 11.859 18.971 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 11.859 18.971 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 11.859 18.971 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 11.859 18.971 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 11.859 18.971 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 11.390 20.219 17.592 1.00 10.37					13	3 15.911				
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ATOM 1074 C THR 133 14.003 13.738 10.00 18.31 ATOM 1075 O THR 133 12.976 13.052 18.539 1.00 14.08 ATOM 1076 N LYS 134 13.992 15.065 18.681 1.00 14.08 ATOM 1077 CA LYS 134 12.738 15.763 18.943 1.00 14.05 ATOM 1078 CB LYS 134 13.028 17.072 19.683 1.00 16.10 ATOM 1079 CG LYS 134 13.566 16.783 21.105 1.00 21.50 ATOM 1080 CD LYS 134 13.739 18.052 21.912 1.00 24.72 ATOM 1081 CE LYS 134 13.962 17.851 23.411 1.00 29.07 ATOM 1082 NZ LYS 134 15.380 17.498 23.673 1.00 35.66 ATOM 1083 C LYS 134 11.982 16.084 17.673 1.00 11.72 ATOM 1083 C LYS 134 10.764 16.268 17.697 1.00 12.75 ATOM 1085 N HIS 135 12.768 16.210 16.602 1.00 10.34 ATOM 1085 CA HIS 135 12.229 16.559 15.278 1.00 9.70 ATOM 1087 CB HIS 135 12.568 18.014 14.927 1.00 10.46 ATOM 1088 CG HIS 135 10.625 19.519 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 10.625 19.519 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 12.334 19.405 17.077 1.00 13.42 ATOM 1089 CD2 HIS 135 12.334 19.405 17.077 1.00 13.42					13	3 17.200				14.81
ATOM 1075 O THR 133 12.976 13.052 18.681 1.00 14.08 ATOM 1076 N LYS 134 13.992 15.065 18.681 1.00 14.05 ATOM 1077 CA LYS 134 12.738 15.763 18.943 1.00 16.10 ATOM 1078 CB LYS 134 13.028 17.072 19.683 1.00 21.50 ATOM 1079 CG LYS 134 13.566 16.783 21.105 1.00 21.50 ATOM 1080 CD LYS 134 13.739 18.052 21.912 1.00 24.72 ATOM 1081 CE LYS 134 13.962 17.851 23.411 1.00 29.07 ATOM 1082 NZ LYS 134 15.380 17.498 23.673 1.00 35.66 ATOM 1082 NZ LYS 134 11.982 16.084 17.673 1.00 11.72 ATOM 1083 C LYS 134 10.764 16.268 17.697 1.00 12.75 ATOM 1085 N HIS 135 12.768 16.210 16.602 1.00 10.34 ATOM 1085 N HIS 135 12.229 16.559 15.278 1.00 9.70 ATOM 1086 CA HIS 135 12.229 16.559 15.278 1.00 9.70 ATOM 1087 CB HIS 135 12.568 18.014 14.927 1.00 10.46 ATOM 1088 CG HIS 135 10.625 19.519 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 10.625 19.519 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 10.625 19.519 15.664 1.00 11.74 ATOM 1089 CD2 HIS 135 12.334 19.405 17.077 1.00 13.42					13					
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ATOM	1092	NES	HIS	13	5 10.358	20 261			
ATOM	1093	С	HIS	13		20.261 15.614	16.753	1.00	14.68
ATOM	1094	0	HIS	13		16.005	14.207	1.00	9.49
MOTA	1095	N	PRO	13		14.336	13.302	1.00	8.95
ATOM	1096	CD	PRO	13		13.714	14.298	1.00	10.29
ATOM	1097	CA	PRO	13		13.348	15.288	1.00	12.71
ATOM	1098	CB	PRO	136			13.367	1.00	10.63
ATOM	1099	CG	PRO	136		12.025	13.738	1.00	13.20
ATOM	1100	С	PRO	136		12.308	14.821	1.00	15.42
ATOM	1101	0	PRO	136		13.656	11.902	1.00	9.37
ATOM	1102	N	GLY	137		13.947	11.540	1.00	10.11
ATOM	1103	CA	GLY	137		13.643	11.131	1.00	9.15
ATOM	1104	С	GLY	137		13.906	9.700	1.00	8.92
ATOM	1105	0	GLY	137		15.351	9.281	1.00	8.41
ATOM	1106	N	PHE	138		15.660	8.076	1.00	8.62
ATOM	1107	CA	PHE	138		16.290	10.230	1.00	7.77
MOTA	1108	CB	PHE	138		17.683	9.858	1.00	7.53
ATOM	1109	CG	PHE	138		18.533	11.069	1.00	9.20
ATOM	1110	CD1	PHE	138		20.014	10.773	1.00	8.61
ATOM	1111	CD2	PHE	138		20.502	9.999	1.00	8.98
ATOM	1112	CE1	PHE	138	11.598	20.897	11.264	1.00	8.98
ATOM	1113	CE2	PHE	138	13.584	21.878	9.728	1.00	9.14
ATOM	1114	CZ	PHE	138	12.555	22.238	11.007	1.00	9.39
ATOM	1115	С	PHE	138	14.355	22.730	10.231	1.00	8.60
ATOM	1116	0	PHE	138		18.318	9.123	1.00	6.57
ATOM	1117	N	GLN	139	14.155	18.953	8.090	1.00	6.31
ATOM	1118	CA	GLN	139	15.553	18.234	9.700	1.00	7.35
ATOM	1119	CB	GLN	139	16.718	18.827	9.045	1.00	7.49
ATOM	1120	CG	GLN	139	17.990	18.600	9.867	1.00	7.76
ATOM	1121	CD	GLN	139	19.211	19.123	9.164	1.00	8.03
ATOM	1.122	OE1	GLN	139	20.475	19.034	10.008	1.00	9.61
ATOM	1123	NE2	GLN	139	20.452	18.629	11.194	1.00	11.81
ATOM	1124	C	GLN	139	21.556	19.403	9.361	1.00	10.42
ATOM	1125	o	GLN	139	16.898	18.263	7.634	1.00	6.36
ATOM	1126	N	ASP	140	17.148	19.042	6.703	1.00	6.70
ATOM	1127	CA	ASP	140	16.792	16.962	7.476	1.00	7.41
ATOM	1128	CB	ASP	140	16.966	16.359	6.153	1.00	8.02
ATOM	1129	CG	ASP	140	17.014	14.845	6.267	1.00	10.06
ATOM	1130	OD1	ASP	140	18.185	14.414	7.143	1.00	12.56
ATOM	1131	OD2	ASP	140	19.263	15.008	7.017	1.00	15.40
ATOM	1132	C	ASP	140	18.010	13.419	7.863	1.00	17.99
ATOM	1133	0	ASP	140	15.903 16.195	16.836	5.173	1.00	7.03
ATOM	1134	N	PHE	141	14.649	17.125	4.012	1.00	7.37
ATOM	1135	CA	PHE	141	13.592	16.886	5.632	1.00	6.76
ATOM	1136	CB	PHE	141	12.241	17.404	4.806	1.00	6.92
MOTA	1137	CG	PHE	141	11.180	17.315	5.525	1.00	8.28
ATOM	1138	CD1	PHE	141	10.649	18.059	4.700	1.00	10.59
ATOM	1139	CD2	PHE	141	10.766	17.398	3.585	1.00	12.85
ATOM	1140	CEl	PHE	141	9.773	19.326	4.979	1.00	12.09
ATOM	1141	CE2	PHE	141	9.946	18.045	2.730	1.00	14.79
ATOM	1142	CZ	PHE	141	9.514	20.027	4.097	1.00	12.80
ATOM	1143	С	PHE	141	13.898	19.385	2.960	1.00	15.56
ATOM	1144	0	PHE	141	13.038	18.843	4.381	1.00	6.10
ATOM	1145	N	ALA	142	14.235	19.227	3.224	1.00	5.52
ATOM	1146	CA	ALA	142	14.436	19.692	5.355	1.00	5.91
ATOM	1147	CB	ALA	142	14.597	21.113	5.109	1.00	6.07
ATOM	1148	C	ALA	142	15.593	21.835	6.444	1.00	6.15
ATOM	1149	0	ALA	142	15.534	21.396	4.153	1.00	5.38
ATOM	1150	N	GLU	143	16.660	22.273	3.289	1.00	5.69
ATOM	1151	CA	GLU	143	17.811	20.630	4.306	1.00	5.79
ATOM	1152	CB	GLU	143	19.021	20.759	3.404	1.00	5.89
ATOM	1153	CG	GLU	143	19.647	19.977	3.912	1.00	6.66
ATOM	1154	CD	GLU	143	20.818	20.589	5.171	1.00	6.49
ATOM	1155	OE1	GLU	143		19.857	5.742	1.00	8.57
ATOM	1156	OE2	GLU	143	20.986 21.529	18.661	5.468	1.00	15.50
ATOM	1157	C	GLU	143		20.401	6.607	1.00	8.03
ATOM	1158		GLU	143	17.426	20.335	1.982	1.00	6.15
ATOM	1159		GLN		17.798	21.030	1.046	1.00	6.03
ATOM	1160		GLN		16.717	19.195	1.852	1.00	6.24
ATOM	1161		GLN		16.249 15.582	18.793	0.519	1.00	5.81
ATOM	1162		GLN			17.418	0.622	1.00	7.33
ATOM	1163		GLN		15.034 16.102	16.900	-0.718	1.00	9.38
ATOM	1164		GLN		16.102	16.723	-1.755	1.00	11.31
					~0.103	17.336	-2.852	1.00	15.13

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						- 95 -				13.37
				144	17.01	7 19	.794	-1.443	1.00	6.08
ATOM	1165		GLN	144	15.32	_	.843	-0.068	1.00	6.65
ATOM	1166	С	GLN	144	15.36).113	-1.286	1.00	5.44
ATOM	1167	0	GLN	145	14.45	0 20	0.464	0.723	1.00	5.36
ATOM	1168	N	TYR	145	13.55	2 2	1.492	0.249	1.00	5.45
ATOM	1169	CA	TYR	145	12.56	2 2	1.956	1.318	1.00	5.34
ATOM	1170	CB	TYR	145	11.7	L8 2	3.094	0.785	1.00	5.77
ATOM	1171	CG	TYR		10.89	_	2.844	-0.266	1.00	5.40
ATOM	1172	CD1	TYR	145	10.1		3.856	-0.832	1.00	6.05
ATOM	1173	CEI	TYR	145	11.8	_	4.392	1.209		5.52
ATOM	1174	CD2	TYR	145	11.1		5.428	0.632	1.00	4.90
ATOM	1175	CE2	TYR	145	10.2		5.146	-0.376	1.00 1.00	6.57
MOTA	1176	CZ	TYR	145	9.5		26.126	-1.002		4.85
ATOM	1177	OH	TYR	145	14.3		22.668	-0.324	1.00	5.67
ATOM	1178	C	TYR	145	14.0		23.173	-1.384	1.00	5.22
MOTA	1179	0	TYR	145	15.4		23.055	0.370	1.00 1.00	5.07
ATOM	1180	N	TYR	146	16.2		24.134	-0.108		6.31
ATOM	1181	CA	TYR	146	17.4		24.302	0.818	1.00 1.00	5.63
ATOM	1182	ÇB	TYR	146	18.		25.533	0.554		4.93
ATOM	1183	CG	TYR	146	18.		26.654	1.367	1.00	4.66
ATOM	1184	CD1	TYR	146	18.		27.804	1.191	1.00	5.91
ATOM	1185	CEl	TYR	146	_		25.595	-0.471	1.00	5.60
	1186	CD2	TYR	146		050	26.728	-0.673	1.00	5.33
MOTA	1187	CE2	TYR	146	_		27.816	0.151	1.00	6.01
MOTA	1188	CZ	TYR	146		892	28.929	-0.076	1.00	4.88
ATOM	1189	OH	TYR	146		681	23.831	-1.547	1.00	5.89
ATOM	1190	C	TYR	146		.740 .630	24.691	-2.413	1.00	5.20
MOTA	1191	0	TYR	146	_		22.580	-1.792	1.00	5.95
ATOM	1192	N	TRP	14	_	.186 .650	22.244	-3.129	1.00	6.61
MOTA	1193	CA	TRP	14			20.995	-3.105	1.00	6.71
ATOM	1194	CB	TRP	14		.544	21.259	-2.221	1.00	6.87
ATOM	1195	CG	TRP	14		.730	22.345	-2.390	1.00	7.71
MOTA	1196	CD2	TRP	14		.675	22.227	-1.334	1.00	7.63
MOTA	1197	CE2	TRP	14		.598	23.398	-3.303	1.00	7.42
MOTA	1198	CE	TRP	14		.828	20.576	-1.120	1.00	
MOTA	1199	CD:		14		127	21.118	-0.574	1.00	7.49
MOTA	1200	NE		1.4		L.230	23.133	~1.198	1.00	8.32 8.76
MOTA	1201	CZ				2.641	24.299	-3.147	1.00	
MOTA	1202	CZ			•	1.873	24.162	2.079	1.00	8.40
MOTA	1203	CH		1	•	2.774	22.124	-4.123	1.00	5.56
ATOM	1203	C	TRP	1		6.514	22.484	-5.295	1.00	6.90 5.62
MOTA	1204	_	TRP		-	6.697	21.663	-3.736	1.00	
MOTA	1205		ASP	1		5.333	21.610	-4.644	1.00	6.73
MOTA	1207		ASE			4.192	20.892	-3.990	1.00	7.41
MOTA	1207					3.006	19.397	-3.794	1.00	9.94 11.03
MOTA	1209					13.180	18.824	-4.385	1.00	
MOTA	1210		D1 ASI	•		14.107	18.805	-3.115	1.00	12.94
MOTA	121		D2 AS	-		12.308	23.013	-5.076	1.00	
MOTA	121	_		-		13.807	23.288	-6.281	1.00	
MOTA	121			-		13.602	23.250	-4.112	1.00	
MOTA	121			L		13.678	25.330	-4.472	1.00	- 10
MOTA	121		A VA	L	149	13.287	26.047	-3.279	1.00	- 05
ATOM	121		B VA	L	149	12.664	26.460	2 202	1.00	4 82
MOTA	121		G1 V	T	149	13.656	27.265		1.00	
MOTA	121		CG2 V	ΛL.	149	11.883	26.084		1.0	
MOTA	123			ΑL	149	14.421	26.951		1.0	
MOTA	123			AL.	149	14.173	25.750		1.0	- 00
MOTA				HE	150	15.669	26.26		1.0	4 6 1
MOTA	12: 12			HE	150	16.795			1.0	- ^ ^ 4
MOTA				HE	150	18.111			1.0	
MOTA	12			HE	150	19.374		•	1.0	
MOTA				HE	150	20.158		•		7.41
MOTA		25	C -	HE	150	19.840		- 03'		00 7.77
MOTA		26		HE	150	21.279				00 8.49
MOTA	•	227		HE	150	20.926	01			00 7.48
MOTA	•	228		PHE	150	21.686	00	- 10		00 5.89
MOTA	•	229	~-	PHE	150	16.61		0.00		00 6.52
MOTA	•	230	•	PHE	150	16.84	1 26.77	7 75	•	00 6.70
MOTA	•	231	•	GLY	151	16.27	6 24.6	0.74		00 6.74
MOTA	•	232	••	GLY	151	16.12	4 24.1	0 4-	16 1.	.00 6.45
ATO	м 1	233	CA	GLY	151	15.01	.2 24.8	30 6	•	.00 7.27
ATO!	M 1	.234	С	GLY	151	15.15	0 25.2		_	.00 6.82
OTA	м 1	235	0 .	LEU	152		7 25.0	0.4	_	.00 6.24
OTA	m I	L236	N	LEU	152		37 25.8	378 -3.4		
ATO		1237	CA							

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						- 96 -				
ATOM		3.8	CB L	EU	152					
ATOM	12	39		EU		. 582	25.881	-8.452	1.00	
ATOM	12	40	_	EU		.452	26.859	-8.828		0.25
ATOM	12	41		EU EU		. 864	26.532	-10.214	1.00	7.23
ATOM	12					.358	26.832	-7.763	1.00	2.15
ATOM	12				152 13	.269	27.298	-9.669	1.00	7.05
ATOM	12				152 13	.015	27.864	-10.743	1.00	6.42
ATOM	124						27.874	-8.702	1.00	7.31
ATOM	124				153 14	.442	29.262	-8.845	1.00	5.98
ATOM	124		CB SE		153 15.	.068	29.742		1.00	6.16
ATOM			OG SE		153 14.		29.755	-7.541	1.00	6.44
ATOM	124		C SE				9.413	-6.522	1.00	6.18
ATOM	124		O SE				0.420	-10.000	1.00	6.14
ATOM	125		N SE	R j		-	8.436	-10.740	1.00	6.53
ATOM	125		CA SE	R 1	54 17.	•	8.495	-10.217	1.00	6.45
ATOM	125	-	CB SE	R 1	54 18.		7.271	-11.340	1.00	7.39
ATOM	125		OG SE	R 1	54 18.	_	7.292	-11.278	1.00	8.84
ATOM	125			٦ ٦	54 16.			10.189	1.00	13.14
ATOM	125	_		_	54 16.	_	8.472	-12.643	1.00	7.57
	125		ALA		55 15.4		9.253	-13.563	1.00	8.31
ATOM	125	-	A ALA		55 14.5		7.630	-12.737	1.00	6.91
ATOM	1258	_	B ALA		55 13.5		7.622	-13.938	1.00	7.39
ATOM	1259) C					5.520	-13.807	1.00	
ATOM	1260	0	ALA				.964	-14.140	1.00	7.77
ATOM	1261	N	LEU				.538	-15.242	1.00	6.87
ATOM	1262						.547	-13.083	1.00	7.86
ATOM	1263						.860	-13.176	1.00	6.99
ATOM	1264	CG					.279	-11.838		5.86
ATOM	1265	CE					.434	-11.365	1.00	5.92
ATOM	1266	CD		15			.809	-9.936	1.00	5.99
ATOM	1267	C		15		36 30	.596	-12.284	1.00	8.87
ATOM	1268	0	LEU	15		10 31	. 933	-13.642	1.00	11.48
ATOM	1269	И	LEU	15		32.	. 805	-14.447	1.00	6.11
ATOM	1270	CA	LEU	15		4 31.	.880	-13.141	1.00	7.28
ATOM	1271			151	7 15.89	8 32.	863	-13.543	1.00	6.74
ATOM	1272	CB	LEU	157	17.15	2 32.	739		1.00	7.25
ATOM		CG	LEU	157			236	-12.694	1.00	6.79
ATOM	1273	CD:		157			026	-11.250	1.00	7.78
ATOM	1274	CD2	LEU	157			672	-10.580	1.00	8.46
ATOM	1275	С	LEU	157		7 32.	740	-11.145	1.00	9.12
ATOM	1276		LEU	157			740	-15.028	1.00	6.91
ATOM	1277	N	LYS	158	16.14		703	-15.638	1.00	7.24
ATOM	1278	CA	LYS	158	16.339		110	-15.606	1.00	7.38
ATOM	1279	CB	LYS	158	16.381			-17.057	1.00	7.07
ATOM	1280	CG	LYS	158	17.574			-17.407	1.00	9.01
ATOM	1281	CD	LYS	158	17.541			~16.887	1.00	10.48
	1282	CE	LYS	158	18.743	,		-17.122	1.00	13.42
ATOM	1283	NZ	LYS	158	18.743	-		-16.407	1.00	18.16
ATOM	1284	C	LYS	158	15.185	5		-16.586	1.00	18.72
ATOM	1285	0	LYS	158				-17.782	1.00	
ATOM	1286	N	GLY	159	15.447	32.8		-18.770	1.00	7.00
ATOM	1287	CA	GLÝ	159	13.951	32.0		-17.281	1.00	9.09
ATOM	1288	С	GLY	159	12.834	32.7		-17.873	1.00	7.17
ATOM	1289	0	GLY	159	13.038	34.2	52	-17.763	1.00	7.22
ATOM	1290	N	TYR	160	12.756	34.9	73	-18.731	1.00	6.90
MOTA	1291	CA	TYR		13.443	34.7	71	-16.620	1.00	7.59
ATOM	1292	CB	TYR	160	13.674	36.23	30	-16.489	1.00	7.51
ATOM	1293	CG	TYR	160	14.004	36.59	5	-15.059		6.84
ATOM	1294	CD1	TYR	160	12.831	36.75	9	-14.120	1.00	7.03
ATOM	1295	CE1	TYR	160	12.421	35.75	2 .	-13.251	1.00	6.77
ATOM	1296	CD2		160	11.353	35.91	.5	-12.430	1.00	6.69
ATOM	1297	CE2	TYR	160	12.097	37.94		-14.093	1.00	7.61
ATOM	1298	CZ	TYR	160	11.013	38.10		-13.247	1.00	7.26
ATOM	1299		TYR	160	10.643	37.08	_	12.380	1.00	7.77
ATOM	1300	ОН	TYR	160	9.594	37.20			1.00	7.26
ATOM	1300	C	TYR	160	14.756	36.70		11.495	1.00	8.86
ATOM	1301	0	TYR	160	14.653	37.77		17.446	1.00	6.38
ATOM		N	ALA	161	15.849	35.96		18.003	1.00	7.25
ATOM	1303	CA	ALA	161	16.929	36.379		17.537	1.00	7.30
ATOM	1304	CB	ALA	161	18.083	35.387		18.438	1.00	7.63
ATOM	1305	C	ALA	161	16.414	36.456		18.293	1.00	9.13
ATOM	1306	0	ALA	161	16.688	37.458		19.886	1.00	7.60
ATOM	1307	N	LEU		15.755	35.401		20.577	1.00	8.23
ATOM	1308	CA .	LEU		15.234	J3.401		20.331	1.00	7.75
ATOM	1309	CB	LEU		14.537	35.423		21.721	1.00	7.67
ATOM.	1310	CG	LEU		15.447	34.094		22.022	1.00	7.94
				•		32.872	- 2	22.168	1.00	8.36

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			ren	162	14.644	31.593	-22.325	1.00	10.23
MOTA	1311		LEU LEU		16.390	33.093	-23.326	1.00	10.26 7.87
MOTA	1312		LEU		14.256	36.582	-21.871	1.00 1.00	8.10
MOTA	1313 1314		LEU	162	14.228	37.234	-22.926 -20.874	1.00	7.67
MOTA	1314	-	ALA	163	13.396	36.840	-20.874	1.00	8.06
MOTA	1316		ALA	163	12.422	37.934	-19.658	1.00	8.57
MOTA	1317		ALA	163	11.568	37.986	-21.162	1.00	8.14
MOTA MOTA	1318	С	ALA	163	13.122	39.278 40.158	-21.830	1.00	9.20
ATOM	1319	0	ALA	163	12.527	39.445	-20.607	1.00	8.56
ATOM	1320	N	LEU	164	14.320	40.688	-20.710	1.00	8.69
ATOM	1321	CA	LEU	164	15.075 15.881	40.917	-19.409	1.00	9.34
ATOM	1322	CB	LEU	164	15.007	41.231	-18.199	1.00	9.92
MOTA	1323	CG	LEU	164 164	15.707	40.869	-16.893	1.00	11.23
MOTA	1324	CD1	LEU	164	14.532	42.665	-18.193	1.00	11.47 8.43
ATOM	1325	CD2	LEU	164	15.968	40.800	-21.920	1.00	10.53
ATOM	1326	C O	LEU	164	16.728	41.751	-22.068	1.00 1.00	9.22
MOTA	1327	И	GLY	165	15.876	39.849	-22.823	1.00	9.48
MOTA	1328	CA	GLY	165	16.653	39.841	-24.034	1.00	9.17
MOTA	1329 1330	C	GLY	165	18.044	39.299	-23.843 -24.692	1.00	10.21
ATOM	1331	Ö	GLY	165	18.900	39.539	-24.052	1.00	9.48
MOTA	1332	N	LYS	166	18.298	38.579	-22.452	1.00	9.96
MOTA MOTA	1333	CA	LYS	166	19.627	38.033	-20.984	1.00	9.69
ATOM	1334	CB	LYS	166	19.982	38.274 39.708	-20.549	1.00	11.03
ATOM	1335	CG	LYS	166	19.946	40.606	-21.352	1.00	14.43
ATOM	1336	CD	LYS	166	20.825	42.029	-20.820	1.00	18.44
ATOM	1337	CE	LYS	166	20.799 21.480	42.980	-21.738	1.00	27.60
ATOM	1338	NZ	LYS	166 166	19.669	36.535	-22.725	1.00	9.64
ATOM	1339	С	LYS	166	18.611	35.926	-22.985	1.00	11.70 9.56
MOTA	1340	0	LYS	167	20.837	35.917	-22.660	1.00	10.09
MOTA	1341	N	GLU GLU	167	20.979	34.447	-22.758	1.00	12.65
- ATOM	1342	CA	GLU	167	22.436	34.051	-22.993	1.00	22.48
MOTA	1343	CB CG	GLU	167	23.380	34.300	-21.838	1.00 1.00	25.40
MOTA	1344	CD	GLU	167	23.665	33.149	-20.891	1.00	32.34
MOTA	1345	OE1	GLU	167	23.311	31.984	-21.190	1.00	31.11
ATOM	1346 1347	OE2	GLU	167	24.326	33.330	-19.840 -21.438	1.00	9.49
ATOM	1347	C	GLU	167	20.484	33.838	-20.407	1.00	10.35
MOTA	1349	0	GLU	167	20.519	34.524	-21.453	1.00	9.82
ATOM ATOM	1350	N	GLU	168	19.999	32.587 32.071	-20.295	1.00	9.33
ATOM	1351	CA	GLU	168		30.725	-20.586	1.00	10.98
ATOM	1352	CB	GLU	168		29.555	-20.607	1.00	11.58
ATOM	1353	CG	GLU	168		28.248	-20.881	- 1.00	12.24
MOTA	1354	CD	GLU	168		27.191	-20.621	1.00	16.73
MOTA	1355	OE1		168 168		28.209	-21.238	1.00	15.75 9.76
MOTA	1356	OE2		168		31.991	-19.021	1.00	
ATOM	1357	C	GLU	16		31.919	-17.957	1.00	10.27
MOTA	1358	0	ASN	16		31.959	-19.098	1.00	11.83
MOTA	1359	N CA	ASN	16		31.849	-17.894	1.00 1.00	17.37
MOTA	1360	CB	ASN	16		30.962	-18.200	1.00	25.58
MOTA	1361	CG	ASN	16	9 23.037		-18-442	1.00	36.44
ATOM	1362 1363	OD:		16			-19.416 -17.485	1.00	33.88
ATOM	1364	ND		16			-17.342	1.00	10.67
ATOM ATOM	1365	С	ASN	16			-16.423	1.00	10.87
ATOM	1366	0	ASN	16			-17.818	1.00	9.81
ATOM	1367		PHE				-17.397	1.00	9.43
ATOM	1368						- 0 110	1.00	10.54
ATOM	1369	CB			70 21.670 70 21.970			1.00	10.68
MOTA	1370					_		1.00	11.73
MOTA	1371				70 22.97 70 21.24			1.00	11.45
ATOM	1372				70 23.27		-18.325	1.00	13.22 13.30
MOTA	1373				70 21.60		-16.603	1.00	13.73
ATOM	1374		E2 PHI Z PHI		70 22.58	1 40.787		1.00	9.39
MOTA	1379				70 22.46		-15.896	1.00	10.53
MOTA	137				70 23.38		-15.313	1.00 1.00	9.21
MOTA	137			_	71 21.41			1.00	9.20
MOTA	137		A PH		.71 21.32	35.48		1.00	9.39
ATOM	137	_	B PH	_	.71 19.88			1.00	
MOTA	138 138	_	G PH		L71 19.2	70 37.02		1.00	
ATOM	138		D1 PH	E	171 18.1		400	1.00	
ATOM	138		D2 PF		171 19.7	51 38.24	, 123,400		
MOTA									

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ATOM	1384	CE:	l PHE	1	71 17.63	7			
ATOM	1389			_			-15.183	1.00	9.69
ATOM	1386		. –		71 19.208		-13.881	1.00	
MOTA			PHE	1	71 18.138	39.369	-14.774		11.03
	1387	_	PHE	1	71 21.798			1.00	9.32
ATOM	1388	0	PHE	1	71 22.557		-13.158	1.00	9.45
MOTA	1389	N	ALA				-12.160	1.00	10.11
ATOM	1390	•			72 21.386		-13.727	1.00	
ATOM			ALA	1.	72 21.662	31.758	-13.141		8.64
	1391		ALA	17	72 20.995			1.00	9.25
ATOM	1392	C	ALA	17			~13.907	1.00	11.46
ATOM	1393	0	ALA				-12.935	1.00	9.80
ATOM	1394	N		17			-12.017	1.00	
ATOM			ARG	17	73 24.014	32.048	-13.757		9.88
	1395	CA	ARG	17	25.456			1.00	10.46
ATOM	1396	CB	ARG	17			-13.607	1.00	10.74
ATOM	1397	CG	ARG	17		32.377	-14.804	1.00	12.02
ATOM	1398	CD				33.888	-14.845	1.00	14.37
ATOM	1399		ARG	17		34.507	-16.235		
ATOM		NE	ARG	17	3 26.118	35.904	-16.110	1.00	22.60
	1400	CZ	ARG	17		37.054		1.00	29.23
ATOM	1401	NH1	ARG	17			-16.666	1.00	27.71
MOTA	1402	NH2	ARG			37.249	-17.871	1.00	38.25
ATOM	1403	C		17		38.128	-16.092	1.00	
ATOM			ARG	17	3 25.967	32.398	-12.321		20.56
	1404	0	ARG	17.	3 27.059	31.984	-11.891	1.00	10.00
ATOM	1405	N	HIS	174			-11.891	1.00	12.18
ATOM	1406	CA	HIS	174		33.305	-11.671	1.00	8.86
ATOM	1407	CB				33.884	-10.385	1.00	
ATOM			HIS	174		35.380	-10.393	1.00	8.97
	1408	CG	HIS	174	25.986	36.119	-11.478		9.34
ATOM	1409	CD2	HIS	174		36.548		1.00	11.02
ATOM	1410	ND1	HIS	174			-11.356	1.00	13.05
ATOM	1411	CE1	HIS			36.543	-12.686	1.00	15.18
ATOM	1412			174		37.180	-13.306	1.00	
ATOM		NE2	HIS	174	27.575	37.238	-12.505		16.14
	1413	C	HIS	174	24.864	33.267		1.00	17.60
ATOM	1414	0	HIS	174			-9.203	1.00	8.17
ATOM	1415	N	PHE	175		33.704	-8.067	1.00	10.44
ATOM	1416	CA			24.093	32.251	-9.482	1.00	
ATOM			PHE	175	23.230	31.536	-8.516		8.57
	1417	CB	PHE	175	21.772	31.678		1.00	7.07
ATOM	1418	CG	PHE	175	20.743	31.096	-8.967	1.00	7.09
ATOM	1419	CD1	PHE	175	19.888	31.036	-8.020	1.00	6.00
ATOM	1420	CD2	PHE			30.101	-8.409	1.00	6.11
ATOM	1421			175	20.644	31.566	-6.725	1.00	
ATOM		CE1	PHE	175	18.940	29.615	-7.548		6.48
	1422	CE2	PHE	175	19.709	31.073		1.00	7.35
ATOM	1423	CZ	PHE	175	18.834		-5.837	1.00	7.65
ATOM	1424	C	PHE	175		30.096	-6.266	1.00	7.87
ATOM	1425	o			23.686	30.089	-8.421	1.00	
ATOM			PHE	175	23.298	29.250	-9.248		7.96
	1426	N	LYS	176	24.602	29.813		1.00	8.40
ATOM	1427	CA	LYS	176	25.320		-7.494	1.00	7.81
ATOM	1428	CB	LYS	176		28.576	-7.473	1.00	7.94
ATOM	1429	CG	LYS		26.813	28.901	-7.674	1.00	10.84
ATOM				176	27.215	29.556	-8.956		
ATOM	1430	CD	LYS	176	28.584	30.190	-8.877	1.00	15.51
	1431	CE	LYS	176	28.905	31.261		1.00	23.52
ATOM	1432	NZ	LYS	176	28.155		-7. 8 86	1.00	31.75
ATOM	1433	C	LYS			32.528	-7.591	1.00	30.18
ATOM	1434			176	25.206	27.890	-6.114	1.00	
ATOM		0	LYS	176	25.237	28.596	-5.079		7.44
	1435	N	PRO	17 7	25.115	26.568		1.00	7.02
ATOM	1436	CD	PRO	177	25.016	25.639	-6.114	1.00	7.06
ATOM	1437	CA	PRO	177	24.978		-7.241	1.00	8.87
ATOM	1438	CB	PRO			25.874	-4.841	1.00	7.22
ATOM				177	24.960	24.392	-5.244	1.00	
ATOM	1439		PRO	177	24.494	24.351	-6.632		9.12
	1440	С	PRO	177	26.107	26.128	3.055	1.00	12.20
ATOM	1441	0	PRO	177	25.842		-3.866	1.00	6.45
ATOM	1442		ASP			26.133	-2.655	1.00	6.96
ATOM	1443			178	27.355	26.340	-4.296	1.00	
ATOM			ASP	178	28.432	26.494	-3.322		7.00
	1444	CB .	ASP	178	29.784	26.223		1.00	7.82
MOTA	1445	CG .	ASP	178	30.055		-3.996	1.00	7.64
ATOM	1446		ASP	178		24.770	-4.225	1.00	8.62
ATOM	1447				29.305	23.888	-3.752	1.00	
ATOM			ASP	178	31.072	24.504	-4.927		10.49
ATOM	1448		ASP	178	28.418	27.826	-2.624	1.00	9.66
ATOM	1449	0 2	ASP	178	29.053	27.922		1.00	8.41
ATOM	1450	N A	ASP	179	27.747		-1.567	1.00	11.48
ATOM	1451		ASP			28.844	-3.172	1.00	7.61
ATOM	1452			179	27.868	30.160	-2.558	1.00	
ATOM		-	ASP	179	29.017	31.003	-3.110		8.48
	1453		LSP	179	28.896	31.215		1.00	14.39
ATOM	1454	OD1 #	SP		27.769		-4.582	1.00	17.08
ATOM	1455		SP			31.231	-5.087	1.00	18.23
ATOM	1456			1/7	29.974	31.247	~5.214	1.00	
	-130	_ A	SP	179	26.622	30.999	-2.437		29.01
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ATOM	1457	0	ASP	179	26.723	32.118	-1.937	1.00	7.91
ATOM	1458	N	THR	180	25.459	30.574	-2.903	1.00	6.15
ATOM	1459	CA	THR	180	24.291	31.397	-2.818	1.00	5.45
MOTA	1460	CB	THR	180	23.061	30.717	-3.495	1.00	6.14
ATOM	1461	OG1	THR	180	21.933	31.564	-3.275	1.00	6.60
ATOM	1462	CG2	THR	180	22.728	29.384	-2.872	1.00	7.19
ATOM	1463	С	THR	180	23.929	31.823	-1.404	1.00	5.42
MOTA	1464	0	THR	180	23.995	31.022	-0.488 -1.291	1.00 1.00	6.17 5.82
MOTA	1465	N	LEU	181	23.568 23.100	33.098 33.709	-0.086	1.00	5.33
ATOM	1466 1467	CA CB	LEU	181 181	23.535	35.173	0.000	1.00	5.68
ATOM ATOM	1468	CG	LEU	181	25.031	35.342	0.214	1.00	7.12
ATOM	1469	CD1	LEU	181	25.527	36.714	-0.116	1.00	9.05
ATOM	1470	CD2	LEU	181	25.431	34.952	1.631	1.00	9.04
ATOM	1471	С	LEU	181	21.596	33.554	0.126	1.00	5.36
MOTA	1472	0	LEU	181	21.002	34.159	1.018	1.00	5.78
MOTA	1473	N	ALA	182	20.943	32.746	-0.705	1.00	5.62
ATOM	1474	CA	ALA	182	19.499	32.518	-0.607	1.00 1.00	5.07 5.84
MOTA	1475	CB	ALA	182	19.041 19.111	31.560 31.916	-1.713 0.741	1.00	5.26
ATOM	1476	C O	ALA ALA	182 182	19.111	31.152	1.390	1.00	5.11
MOTA MOTA	1477 1478	N	SER	183	17.929	32.266	1.215	1.00	5.45
ATOM	1479	CA	SER	183	17.387	31.766	2.475	1.00	5.43
ATOM	1480	CB	SER	183	17.361	32.908	3.478	1.00	6.48
ATOM	1481	OG	SER	183	16.484	33.920	3.050	1.00	7.39
ATOM	1482	С	SER	183	15.975	31.229	2.287	1.00	5.28
ATOM	1483	0	SER	183	15.220	31.691	1.430	1.00	5.14
MOTA	1484	N	VAL	184	15.624	30.298	3.167	1.00	4.72 4.18
MOTA	1485	CA	VAL	184	14.272	29.833 28.311	3.379 3.410	1.00 1.00	4.10
ATOM	1486	CB	VAL VAL	184 184	14.156 12.784	27.827	3.825	1.00	5.78
ATOM ATOM	1487 1488	CG1 CG2	VAL	184	14.574	27.702	2.084	1.00	5.85
ATOM	1489	C	VAL	184	13.803	30.392	4.728	1.00	4.63
ATOM	1490	ō	VAL	184	14.563	30.341	5.712	1.00	5.58
ATOM	1491	N	VAL	185	12.571	30.872	4.785	1.00	5.40
ATOM	1492	CA	VAL	185	11.960	31.260	6.049	1.00	5.11
MOTA	1493	CB	VAL	185	11.732	32.758	6.222	1.00	5.44
ATOM	1494	CG1	VAL	185	11.355	33.084	7.659 5.824	1.00	7.04 7.05
MOTA	1495	CG2	VAL	185 185	12.974 10.664	33.556 30.482	6.215	1.00	5.37
ATOM	1496	C O	VAL VAL	185	9.793	30.537	5.354	1.00	6.79
ATOM ATOM	1497 1498	N	LEU	186	10.525	29.766	7.340	1.00	5.04
ATOM	1499	CA	LEU	186	9.312	29.030	7.659	1.00	5.37
ATOM	1500	CB	LEU	186	9.608	27.651	8.191	1.00	6.74
ATOM	1501	CG	LEU	186	10.519	26.783	7.329	1.00	7.22
ATOM	1502	CD1	LEU	186	10.783	25.457	8.026	1.00	8.08
MOTA	1503	CD2	LEU	186	9.933	26.589	5.923	1.00	7.11 5.24
ATOM	1504	C	LEU	186	8.512	29.883	8.645 9.854	1.00	6.31
MOTA	1505	0	LEU	186 187	8.777 7.577	29.826 30.701	8.165	1.00	5.56
ATOM ATOM	1506 15 07	N CA	ILE	187	6.864	31.641	9.010	1.00	5.65
ATOM	1508	CB	ILE	187	6.589	32.984	8.305	1.00	6.04
MOTA	1509	CG2	ILE	187	5.916	33.986	9.250	1.00	7.75
ATOM	1510	CG1	ILE	187	7.804	33.601	7.633	1.00	6.80
ATOM	1511	CD1	ILE	187	7.550	34.739	6.667	1.00	7.49
MOTA	1512	C	ILE	187	5.511	31.068	9.440	1.00	6.09
MOTA	1513	0	ILE	187	4.740	30.565	8.617	1.00	6.78 6.56
ATOM	1514	N	ARG	188	5.253	31.145	10.736 11.332	1.00 1.00	6.28
ATOM	1515	CA	ARG	188 188	3.970 4.130	30.800 29.967	12.611	1.00	7.38
ATOM	1516 1517	CB CG	ARG ARG	188	2.799	29.623	13.245	1.00	7.70
ATOM ATOM	1517	CD	ARG	188	2.926	29.038	14.641	1.00	9.29
ATOM	1519	NE	ARG	188	1.588	28.821	15.185	1.00	11.11
ATOM	1520	CZ	ARG	188	1.357	28.454	16.431	1.00	12.61
ATOM	1521	NH1	ARG	188	2.357	28.232	17.264	1.00	16.10
ATOM	1522	NH2	ARG	188	0.090	28.327	16.815	1.00	16.40
ATOM	1523	С	ARG	188	3.224	32.081	11.714	1.00	6.29
MOTA	1524	0	ARG	188	3.714	32.892	12.499	1.00	7.23
MOTA	1525	N	TYR	189	2.053	32.239	11.099	1.00	6.43 6.36
MOTA	1526	CA	TYR	189	1.129	33.301 33.997	11.534 10.302	1.00 1.00	7.87
ATOM	1527	CB	TYR	189 189	0.565 1.432	35.109	9.770	1.00	7.69
ATOM	1528	CG CD1	TYR TYR	189	2.245	34.959	8.649	1.00	8.11
ATOM	1529	CDI.	111	100					

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ATOM	1530	CE1	TYR	189	3.023	36.028	8.202	1.00	8.55
MOTA	1531	CD2	TYR	189	1.433	36.344	10.407	1.00	8.98
MOTA	1532	CE2	TYR	189	2.188	37.415	9.969	1.00	9.17
MOTA	1533	CZ	TYR	189	2.981	37.241	8.841	1.00	8.58
ATOM	1534	ОН	TYR	189	3.728	38.328	8.379	1.00	11.03
MOTA	1535	C	TYR	189	0.033	32.562	12.300	1.00	7.25
ATOM ATOM	1536 1537	0	TYR PRO	189 190	-0.678 -0.137	31.766	11.696	1.00	8.05
ATOM	1538	N CD	PRO	190	0.666	32.811 33.760	13.576 14.412	1.00 1.00	6.97
ATOM	1539	CA	PRO	190	-1.091	32.037	14.367	1.00	7.48 7.93
ATOM	1540	CB	PRO	190	-0.484	32.215	15.773	1.00	9.03
ATOM	1541	CG	PRO	190	-0.032	33.667	15.732	1.00	8.65
ATOM	1542	С	PRO	190	-2.516	32.564	14.390	1.00	7.31
ATOM	1543	0	PRO	190	-2.768	33.746	14.183	1.00	7.83
MOTA	1544	N	TYR	191	-3.428	31.672	14.740	1.00	8.07
MOTA	1545	CA	TYR	191	-4.758	32.035	15.189	1.00	8.05
ATOM ATOM	1546 1547	CB CG	TYR TYR	191 191	-5.741 -7.089	30.882 31.164	15.033 15.645	1.00	9.47
ATOM	1548	CD1	TYR	191	-7.083	32.032	15.052	1.00 1.00	8.74 10.94
ATOM	1549	CE1	TYR	191	-9.203	32.283	15.640	1.00	12.35
ATOM	1550	CD2	TYR	191	-7.434	30.628	16.867	1.00	11.98
ATOM	1551	CE2	TYR	191	-8.662	30.860	17.464	1.00	13.36
MOTA	1552	CZ	TYR	191	-9.520	31.710	16.847	1.00	13.52
ATOM	1553	OH	TYR		-10.758	31.949	17.411	1.00	20.40
ATOM	1554	С	TYR	191	-4.634	32.352	16.687	1.00	8.41
MOTA	1555	0	TYR	191	-4.028	31.574	17.419	1.00	10.11
ATOM	1556	N	LEU	192	-5.188 -5.170	33.493	17.089	1.00	9.02
ATOM ATOM	1557 1558	CA CB	LEU	192 192	-4.106	33.90 1 35.000	18.490 18.751	1.00	9.80 10.70
ATOM	1559	CG	LEU	192	-2.670	34.624	18.449	1.00	11.38
ATOM	1560	CD1	LEU	192	-1.779	35.835	18.366	1.00	15.17
ATOM	1561	CD2	LEU	192	-2.195	33.545	19.376	1.00	14.95
ATOM	1562	C	LEU	192	-6.524	34.466	18.870	1.00	11.59
ATOM	1563	0	LEU	192	-7.087	35.298	18.167	1.00	13.64
ATOM	1564	N	ASP	193	-7.038	34.106	20.036	1.00	14.51
ATOM	1565	CA	ASP	193	-8.305	34.590	20.567	1.00	17.44
ATOM ATOM	1566	С 0	ASP ASP	193 193	-8.162	34.839	22.054	1.00	18.14
ATOM	1567 156 8	CB	ASP	193	-8.094 -9.424	33.884 33.558	22.833 20.361	1.00	20.69 19.90
ATOM	1569	CG	ASP		-10.778	34.035	20.844	1.00	22.56
ATOM	1570	OD1	ASP		10.950	35.239	21.071	1.00	31.28
ATOM	1571	OD2	ASP		11.705	33.195	20.904	1.00	31.66
ATOM	1572	N	PRO	194	-8.007	36.055	22.502	1.00	19.75
ATOM	1573	CD	PRO	194	~7.751	36.353	23.938	1.00	21.02
ATOM	1574	CA	PRO	194	-8.074	37.262	21.705	1.00	20.34
ATOM	1575	CB	PRO	194	-8.358	38.337	22.780	1.00	22.22
ATOM ATOM	1576 1577	CG C	PRO PRO	194 194	-7.623 -6.794	37.846	23.976 20.961	1.00	23.24
ATOM	1578	0	PRO	194	-5.732	37.553 37.174	21.441	1.00	18.30 20.47
ATOM	1579	N	TYR	195	-6.908	38.261	19.844	1.00	16.09
ATOM	1580	CA	TYR	195	-5.729	38.654	19.057	1.00	13.39
ATOM	1581	CB	TYR	195	-6.063	38.748	17.591	1.00	11.89
MOTA	1582	CG	TYR	195	-4.857	38.589	16.678	1.00	10.40
ATOM	1583	CD1	TYR	195	-4.733	37.428	15.902	1.00	9.05
ATOM	1584	CE1	TYR	195	-3.668	37.229	15.052	1.00	9.43
ATOM	1585	CD2	TYR	195	-3.867	39.556	16.532	1.00	11.25
ATOM ATOM	1586 1587	CE2 CZ	TYR TYR	195 195	-2.801 -2.706	39.370 38.217	15.678 14.940	1.00	10.47
ATOM	1588	OH	TYR	195	-1.631	38.037	14.940	1.00 1.00	9.27 10.15
ATOM	1589	C	TYR	195	-5.251	40.015	19.570	1.00	16.02
ATOM	1590	0	TYR	195	-6.045	40.984	19.547	1.00	19.50
ATOM	1591	N	PRO	196	-4.015	40.101	20.038	1.00	19.81
ATOM	1592	CD	PRO	196	-2.943	39.107	19.944	1.00	20.75
ATOM	1593	CA	PRO	196	-3.555	41.366	20.632	1.00	22.65
ATOM	1594	CB	PRO	196	-2.113	41.061	21.050	1.00	24.78
ATOM	1595	CG	PRO	196	-1.702	39.919	20.178	1.00	25.22
ATOM	1596	C	PRO	196	-3.528	42.534	19.659	1.00	21.80
ATOM ATOM	1597 1598	O N	PRO ALA	196 197	-2.893 -4.121	42.411	18.610 20.069	1.00	18.33
ATOM	1598	CA	ALA	197	-4.121	43.655 44.850	19.209	1.00 1.00	20.80 17.10
ATOM	1600	CB	ALA	197	-4.992	45.932	19.209	1.00	22.74
ATOM	1601	C .	ALA	197	-2.736	45.332	18.943	1.00	16.42
ATOM	1602	0	ALA	197	-2.416	45.845	17.884	1.00	14.48

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ATOM	1603	N	ALA	198	-1.806	45.093	19.872	1.00	13.94
ATOM	1604	CA	ALA	198		45.551	19.663	1.00	18.82
ATOM ATOM	1605 1606	CB C	ALA	198		45.537	20.917	1.00	21.76
ATOM	1607	0	ALA ALA	198 198	0.247	44.830	18.532	1.00	20.09
ATOM	1608	N	ALA	198	1.209 -0.282	45.380	17.989	1.00	20.87
MOTA	1609	CA	ALA	199	0.284	43.655 42.883	18.148	1.00	18.02
ATOM	1610	СВ	ALA	199	0.131	41.377	17.055 17.305	1.00	20.04
ATOM	1611	C	ALA	199	-0.405	43.201	15.745	1.00 1.00	22.29
ATOM	1612	0	ALA	199	-0.143	42.526	14.746	1.00	17.65 19.33
MOTA	1613	И	ILE	200	-1.272	44.187	15.758	1.00	14.55
ATOM	1614	CA	ILE	200	-2.007	44.619	14.572	1.00	12.89
MOTA	1615	CB	ILE	200	-3.524	44.490	14.735	1.00	12.11
ATOM ATOM	1616	CG2	ILE	200	-4.273	44.933	13.481	1.00	15.92
ATOM	1617 1618	CG1 CD1	ILE	200	-3.933	43.079	15.169	1.00	12.87
MOTA	1619	C	ILE	200 200	-5.369	42.887	15.559	1.00	15.12
ATOM	1620	0	ILE	200	-1.604 -1.722	46.049 46.945	14.242	1.00	12.80
ATOM	1621	N	LYS	201	-1.079	46.217	15.061 13.030	1.00	15.14
ATOM	1622	CA	LYS	201	-0.723	47.561	12.585	1.00	12.46
ATOM	1623	C	LYS	201	-1.842	48.108	11.711	1.00 1.00	13.42
ATOM	1624	0	LYS	201	-2.682	47.341	11.198	1.00	12.82 12.98
ATOM	1625	CB	LYS	201	0.575	47.555	11.793	1.00	15.55
ATOM	1626	CG	LYS	201	1.786	47.469	12.720	1.00	22.73
ATOM	1627	CD	LYS	201	2.968	47.442	11.792	1.00	30.21
ATOM	1628	CE	LYS	201	3.330	45.969	11.633	1.00	33.55
ATOM	1629	NZ	LYS	201	4.352	45.602	12.674	1.00	44.14
ATOM ATOM	1630	N	THR	202	-1.844	49.414	11.525	1.00	12.30
ATOM	1631 1632	CA CB	THR THR	202	-2.896	50.018	10.731	1.00	12.03
ATOM	1633	OG1	THR	202 202	-3.769 -4.283	50.900	11.654	1.00	14.94
ATOM	1634	CG2	THR	202	-4.263	50.136 51.401	12.749	1.00	20.93
ATOM	1635	C	THR	202	-2.353	50.883	10.876 9.608	1.00	16.31
ATOM	1636	0	THR	202	-1.574	51.831	9.881	1.00	10.86
ATOM	1637	N	ALA	203	-2.710	50.593	8.362	1.00	12.79 10.61
ATOM	1638	CA	ALA	203	-2.246	51.412	7.251	1.00	10.61
ATOM	1639	CB	ALA	203	-2.554	50.704	5.923	1.00	10.92
ATOM	1640	С	ALA	203	-2.907	52.771	7.177	1.00	11.45
ATOM	1641	0	ALA	203	-3.927	53.003	7.798	1.00	12.75
ATOM ATOM	1642	И	ALA	204	-2.316	53.701	6.418	1.00	13.11
ATOM	1643 1644	CA CB	ALA ALA	204	-2.922	55.016	6.262	1.00	14.24
ATOM	1645	C	ALA	204 204	-2.081 -4.312	55.921	5.383	1.00	17.62
ATOM	1646	ō	ALA	204	-5.116	54.951 55.828	5.666	1.00	15.18
ATOM	1647	N	ASP	205	-4.656	53.935	5.979 4.910	1.00	18.40
ATOM	1648	CA	ASP	205	-6.010	53.765	4.378	1.00	14.70 15.08
ATOM	1649	CB	ASP	205	-5.939	53.130	2.979	1.00	14.53
ATOM	1650	CG	ASP	205	-5.558	51.681	2.919	1.00	13.86
ATOM	1651	OD1	ASP	205	-5.431	51.036	3.978	1.00	13.58
ATOM	1652	OD2	ASP	205	-5.414	51.137	1.785	1.00	14.56
ATOM ATOM	1653	C	ASP	205	-6.958	53.042	5.330	1.00	13.99
ATOM	1654	0	ASP	205	-8.100	52.729	4.944	1.00	16.91
ATOM	1655 1656	N CA	GLY GLY	206	-6.470	52.672	6.523	1.00	13.46
ATOM	1657	C	GLY	206 206	-7.305 -7.215	51.999	7.498	1.00	13.34
ATOM	1658	ō	GLY	206	-7.688	50.496 49.850	7.536	1.00	12.65
ATOM	1659	N	THR	207	-6.523	49.909	8.492 6.562	1.00 1.00	15.08
ATOM	1660	CA	THR	207	-6.383	48.461	6.501	1.00	11.08 10.33
ATOM	1661	CB	THR	207	-5.728	48.047	5.186	1.00	10.43
MOTA	1662	OG1.	THR	207	-6.475	48.593	4.068	1.00	11.13
ATOM	1663	CG2	THR	207	-5.730	46.528	5.000	1.00	11.62
ATOM	1664	С	THR	207	-5.542	47.948	7.669	1.00	10.83
ATOM	1665	0	THR	207	-4.460	48.451	7.944	1.00	11.23
ATOM ATOM	1666	N	LYS	208	-6.047	46.906	8.322	1.00	10.43
ATOM	1667 1668	CA CB	LYS	208	-5.328	46.251	9.393	1.00	10.06
ATOM	1669	CG	LYS LYS	208 208	-6.299 -7.310	45.472	10.281	1.00	10.90
ATOM	1670	CD	LYS	208	-7.310 -8.216	46.400	10.977	1.00	15.45
ATOM	1671	CE	LYS	208	-8.216 -9.070	45.550 46.277	11.860 12.858	1.00	21.10
ATOM	1672	NZ	LYS		10.228	45.455	13.309	1.00 1.00	25.92
ATOM	1673	C	LYS	208	-4.281	45.341	8.753	1.00	35.34 8.69
ATOM	1674	0	LYS	208	-4.631	44.523	7.893	1.00	8.73
ATOM	1675	N	LEU	209	-3.058	45.470	9.211	1.00	8.66
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		<i>~</i> 3	1 511	209	-1.912	44.745	8.686	1.00	8.20
MOTA	1676	CA CB	LEU		-0.919	45.780	8.126	1.00	8.17
MOTA	1677	CG	LEU		-1.407	46.777	7.084	1.00	8.96
ATOM	1678 1679	CD1	LEU		-0.263	47.711	6.737	1.00	10.26
ATOM ATOM	1680	CD2	LEU	209	-1.959	46.077	5.837	1.00	9.92
ATOM	1681	C	LEU	209	-1.149	43.969	9.733	1.00	8.39
ATOM	1682	0	LEU	209	-1.077	44.308	10.910	1.00	9.60 7.50
ATOM	1683	N	SER	210	-0.445	42.944	9.250	1.00	8.27
ATOM	1684	CA	SER	210	0.555	42.241	10.017 9.879	1.00 1.00	9.13
MOTA	1685	CB	SER	210	0.481	40.717	10.458	1.00	10.38
MOTA	1686	OG	SER	210	-0.677	40.154 42.709	9.625	1.00	8.82
ATOM	1687	С	SER	210	1.958	42.709	10.430	1.00	11.07
MOTA	1688	0	SER	210	2.867 2.153	43.228	8.404	1.00	8.41
MOTA	1689	N	PHE	211 211	3.465	43.640	7.944	1.00	8.42
ATOM	1690	CA CB	PHE PHE	211	4.294	42.502	7.351	1.00	9.04
ATOM	1691	CG	PHE	211	5.784	42.797	7.169	1.00	8.29
ATOM	1692 1693	CD1	PHE	211	6.656	42.844	8.237	1.00	9.90
ATOM ATOM	1694	CD2	PHE	211	6.316	43.023	5.916	1.00	8.43
ATOM	1695	CEl	PHE	211	8.014	43.064	8.074	1.00	9.71 9.43
ATOM	1696	CE2	PHE	211	7.649	43.256	5.735	1.00	8.86
ATOM	1697	CZ	PHE	211	8.515	43.240	6.804	1.00 1.00	7.66
ATOM	1698	С	PHE	211	3.249	44.762	6.938	1.00	8.72
ATOM	1699	0	PHE	211	2.415	44.662	6.051 7.143	1.00	7.99
ATOM	1700	N	GLU	212	3.963	45.856	6.365	1.00	7.78
MOTA	1701	CA	GLU	212	3.752	47.072 48.319	7.076	1.00	10.35
MOTA	1702	CB	GLU	212	4.267 3.201	49.142	7.809	1.00	15.96
MOTA	1703	CG	GLU	212 212	2.280	49.935	6.895	1.00	17.40
MOTA	1704	CD	GLU GLU	212	1.606	50.866	7.415	1.00	19.49
MOTA	1705	OE1 OE2	GLU	212	2.214	49.708	5.623	1.00	15.01
MOTA	1706 1707	C	GLU	212	4.328	46.972	4.954	1.00	7.86
ATOM ATOM	1707	0	GLU	212	5.006	46.040	4.555	1.00	8.28
ATOM	1709	N	TRP	213	3.992	47.997	4.162	1.00	8.57
ATOM	1710	ÇA	TRP	213	4.464	48.141	2.806	1.00	8.31
ATOM	1711	CB	TRP	213	3.999	49.421	2.155	1.00 1.00	9.80
ATOM	1712	CG	TRP	213	4.620	50.707	2.603 2.074	1.00	11.28
ATOM	1713	CD2	TRP	213	5.776	51.317	2.784	1.00	12.37
ATOM '	1714	CE2	TRP	213	5.977	52.520 50.973	1.031	1.00	12.51
MOTA	1715	CE3	TRP	213	6.644 4.181	51.522	3.610	1.00	10.15
ATOM	1716	CD1	TRP TRP	213 213	4.101	52.619	3.734	1.00	12.18
MOTA	1717	NE1	TRP	213	7.053	53.363	2.474	1.00	14.69
MOTA	1718	CZ2 CZ3	TRP	213	7.687	51.805	0.735	1.00	13.88
ATOM	1719 1720	CH2	TRP	213	7.887	52.990	1.460	1.00	15.53
ATOM ATOM	1721	C	TRP	213	5.991	48.089	2.741	1.00	7.51
ATOM	1722	O	TRP	213	6.720	48.548	3.592	1.00	8.44 7.74
ATOM	1723	N	HIS	214	6.470	47.422	1.657	1.00	7.66
ATOM	1724	CA	HIS	214	7.890	47.280	1.443 2.447	1.00	7.45
ATOM	1725	CB	HIS	214	8.495	46.246	2.273	1.00	7.38
MOTA	1726	CG	HIS	214	7.976	44.860 43.765	1.682	1.00	7.28
MOTA	1727	CD2	HIS	214	8.527 6.682	44.495	2.637	1.00	6.92
ATOM	1728	ND1	HIS	214 214	6.501	43.234	2.298	1.00	7.44
ATOM	1729	CE1		214	7.581	42.759	1.734	1.00	7.83
MOTA	1730	NE2 C	HIS	214	8.125	46.789	0.014	1.00	6.97
ATOM	1731	0	HIS	214	7.212	46.319	-0.642	1.00	7.95
ATOM	1732 1733	N	GLU	215		46.910	-0.408	1.00	7.78
MOTA MOTA	1734	CA	GLU	215	9.921	46.216	-1.569	1.00	8.05
ATOM	1735	CB	GLU	215	10.780	47.140	-2.413	1.00	9.46 11.54
ATOM	1736	CG	GLU	215		48.276	-3.051	1.00 1.00	16.19
MOTA	1737	CD	GLU	215		49.189	-3.900	1.00	15.97
ATOM	1738	OEI		215		49.042	-3.934 -4.616	1.00	23.46
ATOM	1739	QE2		215		50.051 45.070	-1.025	1.00	8.11
ATOM	1740	С	GLU	215		45.184	0.071	1.00	8.95
MOTA	1741	0	GLU	215		43.985	-1.761	1.00	7.98
ATOM	1742	N	ASP ASP	216 216		42.873	-1.305	1.00	6.84
ATOM	1743	CA	ASP	216		41.564	-1.990	1.00	7.14
MOTA	1744	CB CG		216		40.991	-1.580	1.00	6.78
ATOM	1745 1746	DO		216		41.594	-0.693	1.00	7.44
ATOM	1745	OD		21		39.909	-2.098	1.00	7.77
MOTA MOTA	1748	C	ASP	21		43.128	-1.469	1.00	6.24
ALON	27.10	-							

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ATOM	1749	0	ASP	216	13.696	43.704	-2.450	1.00	7.93
ATOM	1750	N	VAL	217	13.931	42.555	-0.509	1.00	6.61
ATOM	1751	CA	VAL	217	15.369	42.439	-0.559	1.00	6.71
ATOM ATOM	1752	CB	VAL	217	16.050	42.687	0.780	1.00	7.87
ATOM	1753 1754	CG1 CG2	VAL VAL	217	17.568	42.640	0.641	1.00	9.01
ATOM	1755	C	VAL	217 217	15.613 15.714	44.001	1.353	1.00	9.65
ATOM	1756	o	VAL	217	15.714	41.072 40.051	-1.150 -0.482	1.00	6.75
ATOM	1757	N	SER	218	15.852	41.047	-2.476	1.00	7.26
ATOM	1758	CA	SER	218	16.056	39.850	-3.257	1.00	6.83 6.43
ATOM	1759	CB	SER	218	14.837	38.910	-3.175	1.00	6.60
MOTA	1760	OG	SER	218	13.749	39.472	-3.890	1.00	6.81
ATOM	1761	C	SER	218	16.304	40.211	-4.722	1.00	5.92
ATOM	1762	0	SER	218	16.044	41.351	-5.112	1.00	6.97
ATOM ATOM	1763 1764	N	LEU	219	16.723	39.209	-5.488	1.00	6.04
ATOM	1765	CA CB	LEU LEU	219 219	16.663	39.294	-6.937	1.00	6.10
ATOM	1766	CG	LEU	219	17.722 17.728	38.393 38.321	-7.569	1.00	6.78
ATOM	1767	CD1	LEU	219	18.034	39.650	-9.097 -9.731	1.00	7.82
ATOM	1768	CD2	LEU	219	18.660	37.225	-9.589	1.00	9.76 8.26
MOTA	1769	C	LEU	219	15.218	36.982	-7.341	1.00	5.92
ATOM	1770	0	LEU	219	14.541	39.784	-7.957	1.00	6.32
ATOM	1771	N	ILE	220	14.743	37.780	-6.965	1.00	5.60
ATOM	1772	CA	ILE	220	13.342	37.411	-7.010	1.00	5.79
ATOM	1773	CB	ILE	220	12.950	36.552	-8.228	1.00	6.51
ATOM ATOM	1774	CG2	ILE	220	13.285	37.295	-9.523	1.00	7.78
ATOM	1775 1776	CG1 CD1	ILE ILE	220 220	13.563	35.144	-8.189	1.00	6.95
ATOM	1777	CDI	ILE	220	13.002 12.977	34. 2 22 36.695	-9.250	1.00	7.96
ATOM	1778	Ö	ILE	220	13.869	36.252	-5.712 -4.968	1.00	5.16
ATOM	1779	N	THR	221	11.694	36.656	-5.419	1.00 1.00	5.70
MOTA	1780	CA	THR	221	11.121	35.981	-4.263	1.00	5.46 6.07
ATOM	1781	CB	THR	221	10.391	36.988	-3.362	1.00	6.78
ATOM	1782	OG1	THR	221	11.360	37.970	-2.958	1.00	6.64
ATOM	1783	CG2	THR	221	9.809	36.316	-2.133	1.00	7.54
ATOM	1784	C	THR	221	10.182	34.891	-4.753	1.00	5.05
ATOM ATOM	1785 1786	O N	THR	221	9.365	35.121	-5.667	1.00	6.03
ATOM	1787	CA	VAL VAL	222 222	10.317 9.635	33.704	-4.181	1.00	5.43
ATOM	1788	CB	VAL	222	10.610	32.477 31.467	-4.589 -5.188	1.00	5.29
ATOM	1789	CG1	VAL	222	9.950	30.168	-5.590	1.00 1.00	5.74 6.07
ATOM	1790	CG2	VAL	222	11.389	32.046	-6.358	1.00	6.22
ATOM	1791	C	VAL	222	8.867	31.924	-3.379	1.00	5.62
ATOM	1792	0	JAV	222	9.466	31.333	-2.465	1.00	5.72
ATOM	1793	N	LEU	223	7.572	32.200	-3.305	1.00	5.40
ATOM	1794	CA	LEU	223	6.799	32.054	-2.080	1.00	5.71
ATOM ATOM	1795 1796	CB CG	LEU	223	6.211	33.454	-1.749	1.00	5.73
ATOM	1797	CD1	LEU LEU	223 223	5.245	33.563	-0.576	1.00	5.62
ATOM	1798	CD2	LEU	223	5.992 4.631	33.305 34.983	0.748	1.00	5.34
ATOM	1799	C	LEU	223	5.672	31.053	-0.564 -2.119	1.00 1.00	7.58
ATOM	1800	0	LEU	223	4.853	31.106	-3.012	1.00	5.89 6.54
ATOM	1801	N	TYR	224	5.637	30.185	-1.112	1.00	5.35
ATOM	1802	CA	TYR	224	4.493	29.307	-0.858	1.00	5.93
ATOM	1803	CB	TYR	224	4.891	27.865	-0.543	1.00	7.37
ATOM	1804	CG	TYR	224	3.696	27.082	-0.030	1.00	8.60
ATOM ATOM	1805	CD1	TYR	224	2.805	26.474	-0.888	1.00	10.86
ATOM	1806 1807	CE1 CD2	TYR	224	1.698	25.762	-0.350	1.00	11.92
ATOM	1808	CE2	TYR TYR	224 224	3.459	26.927	1.341	1.00	10.88
ATOM	1809	CZ	TYR	224	2.363 1.500	26.334 25.717	1.897	1.00	12.37
ATOM	1810	ОН	TYR	224	0.388	25.717	1.012 1.575	1.00	12.52
ATOM	1811	С	TYR	224	3.702	29.956	0.284	1.00 1.00	16.93
ATOM	1812	Ō	TYR	224	4.318	30.259	1.319	1.00	5.19 6.49
ATOM	1813	N	GLN	225	2.391	29.993	0.209	1.00	5.70
ATOM	1814	CA	GLN	225	1.552	30.327	1.336	1.00	6.51
ATOM	1815	CB	GLN	225	1.053	31.753	1.362	1.00	8.15
ATOM	1816	CG	GLN	225	2.113	32.840	1.196	1.00	8.18
ATOM	1817	CD	GLN	225	1.591	34.205	1.582	1.00	8.60
ATOM	1818	OE1	GLN	225	2.147	34.911	2.439	1.00	11.27
ATOM ATOM	1819	NE2	GLN	225	0.536	34.580	0.927	1.00	9.01
ATOM	1820 1821	С 0	GLN GLN	225 225	0.332	29.411	1.366	1.00	7.75
	2041	J	024	663	-0.163	28.937	0.352	1.00	8.52

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MOTA	1822	N	SER	226	-0.198	29.227	2.575	1.00	9.34
ATOM	1823	CA	SER	226	-1.464	28.544	2.758	1.00	10.96
ATOM	1824	CE	SER	226	-2.003	28.665	4.164	1.00	16.30
ATOM	1825	OG	SER	226	-1.115	28.419	5.120	1.00 1.00	15.06 10.35
MOTA	1826	C	SER	226	-2.559	29.310 30.484	2.014 1.699	1.00	11.80
MOTA	1827	0	SER	226	-2.481 -3.684	28.605	1.934	1.00	10.66
ATOM	1828	N	ASN ASN	227 227	-4.840	29.105	1.234	1.00	11.50
ATOM	1829 1830	CA CB	ASN	227	-5.725	27.953	0.769	1.00	15.38
ATOM ATOM	1831	CG	ASN	227	-6.303	28.312	-0.576	1.00	22.10
ATOM	1832	OD1	ASN	227	-6.033	27.643	-1.583	1.00	35.45
ATOM	1833	ND2	ASN	227	-6.869	29.471	-0.713	1.00	20.67
MOTA	1834	C	ASN	227	-5.668	30.072	2.070	1.00	12.61 15.01
ATOM	1835	0	ASN	227	-6.857	29.812	2.296 2.514	1.00 1.00	10.77
ATOM	1836	N	VAL	228	-5.078	31.162 32.223	3.268	1.00	9.90
MOTA	1837	CA	VAL	228 228	-5.746 -5.417	32.223	4.768	1.00	11.72
ATOM	1838 1839	CB CG1	VAL VAL	228	-6.173	33.357	5.454	1.00	14.80
ATOM ATOM	1840	CG2	VAL	228	-5.721	30.872	5.403	1.00	14.80
ATOM	1841	C	VAL	228	-5.284	33.531	2.644	1.00	9.82
ATOM	1842	0	VAL	228	-4.093	33.821	2.657	1.00	10.96
MOTA	1843	N	GLN	229	-6.185	34.288	2.031	1.00	9.94 9.11
ATOM	1844	CA	GLN	229	-5.815	35.512	1.345	1.00 1.00	10.74
ATOM	1845	CB	GLN	229	-7.038	36.050	0.595 -0.481	1.00	10.74
ATOM	1846	CG	GLN	229	-6.750	37.084 38.4 7 9	0.038	1.00	11.49
MOTA	1847	CD	GLN	229 229	-6.454 -7.057	38.953	1.011	1.00	12.74
ATOM	1848	OE1 NE2	GLN GLN	229	-5.440	39.124	-0.556	1.00	10.77
ATOM	1849 1850	C	GLN	229	-5.228	36.489	2.340	1.00	9.22
ATOM ATOM	1851	0	GLN	229	-5.784	36.712	3.421	1.00	10.98
ATOM	1852	N	ASN	230	-4.133	37.140	1.924	1.00	8.54
ATOM	1853	CA	ASN	230	-3.504	38.106	2.839	1.00	9.75
ATOM	1854	CB	ASN	230	-2.642	37.356	3.865	1.00	10.52 11.42
MOTA	1855	CG	ASN	230	-1.468	36.649	3.229	1.00 1.00	12.95
ATOM	1856	OD1	ASN	230	-1.601	35.602	2.559 3.367	1.00	10.36
ATOM	1857	ND2	ASN	230	-0.321 -2.684	37.258 39.17 7	2.186	1.00	9.22
ATOM	1858	C	ASN	230 230	-2.579	40.278	2.699	1.00	10.88
ATOM	1859	N O	ASN LEU	231	-2.080	38.928	1.008	1.00	8.35
MOTA MOTA	1860 1861	CA	LEU	231	-1.187	39.891	0.391	1.00	7.65
MOTA	1862	CB	LEU	231	-0.166	39.130	-0.486	1.00	9.10
ATOM	1863	CG	LEU	231	0.859	38.294	0.253	1.00	10.43
MOTA	1864	CD1	LEU	231	1.718	37.494	-0.719	1.00	12.85
ATOM	1865	CD2	LEU	231	1.707	39.142	1.167	1.00	18.74 7.60
ATOM	1866	C	LEU	231	-1.921	40.933 40.618	-0.444 -1.110	1.00	8.69
ATOM	1867	0	LEU	231	-2.902 -1.378	42.167	-0.446	1.00	7.25
MOTA	1868	N	GLN GLN	232 232	-1.884	43.212	-1.298	1.00	7.79
ATOM	1869	CA CB	GLN	232	-2.611	44.274	-0.523	1.00	8.77
ATOM ATOM	1870 1871	CG	GLN	232	-3.852	43.777	0.218	1.00	8.38
ATOM	1872	CD	GLN	232	-4.616	44.915	0.825	1.00	10.24
ATOM	1873	OE1	GLN	232	-4.059	45.793	1.487	1.00	11.66
ATOM	1874	NE2	GLN	232	-5.935	44.904	0.648	1.00	14.46
MOTA	1875	С	GLN	232	-0.682	43.819	-2.003	1.00 1.00	6.81 7.95
MOTA	1876	0	GLN	232	0.375	43.965	-1.390 -3.244	1.00	7.92
MOTA	1877	N	VAL	233	-0.905	44.246 44.893	-4.061	1.00	8.46
MOTA	1878	CA	VAL	233 233	0.087 0.462	44.130	-5.339	1.00	9.34
ATOM	1879	CB	LAV LAV	233	-0.719	43.775	-6.224	1.00	10.46
ATOM	1880	CG1 CG2	VAL	233	1.534	44.837	-6.141	1.00	9.44
ATOM	1881 1882	C	VAL	233	-0.381	46.307	-4.399	1.00	8.77
ATOM ATOM	1883	ō	VAL	233		46.486	-4.737	1.00	10.72
ATOM	1884	N	GLU	234	0.489	47.302	-4.314	1.00	8.62
MOTA	1885	CA	GLU	234		48.654	-4.763	1.00	10.41
ATOM	1886	CB	GLU	234		49.693	-4.115	1.00	11.08 12.76
ATOM	1887	CG	GLU	234		51.126	-4.319 -3.531	1.00 1.00	13.73
ATOM	1888	CD	GLU	234		52.093 51.97 5	-3.531 -3.567	1.00	16.36
ATOM	1889	OE1		234		53.025	-2.925	1.00	16.64
ATOM	1890	OE2	GLU GLU	234 234		48.736	-6.285	1.00	12.14
ATOM	1891	с 0	GLU	234		48.366	-6.885	1.00	13.51
ATOM	1892 1893	И	THR	235		49.285	-6.917	1.00	15.59
ATOM ATOM	1894	CA	THR	235		49.507	-8.364	1.00	17.29
2701.1	.051								

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							-9.200	1.00	19.13
	1895	CB TH	ir 2	235 -	1.595	48.591	-8.938	1.00	21.58
ATOM	1896		HR 2		-2.984	48.842	-8.952	1.00	22.36
ATOM	1897		HR :	235	-1.375	47.100	-8.576	1.00	18.85
ATOM	1898		HR :	235	-1.137	50.959	-7.579	1.00	19.19
MOTA	1899	-		235	-1.394	51.656	-9.856	1.00	22.89
MOTA		_		236	-1.293	51.330		1.00	23.88
ATOM	1900			236	-1.784	52.664	-10.222	1.00	31.13
ATOM	1901				-1.749	52.894	-11.725	1.00	24.49
MOTA	1902				-3.206	52.889	-9.731	1.00	31.36
ATOM	1903				-3.723	53.962	-9.427	1.00	24.56
ATOM	1904	-			-3.929	51.774	-9.619	1.00	25.87
ATOM	1905		LLA ALA	237	-5.299	51.889	-9.150		33.93
MOTA	1906	-		237	-6.155	50.804	-9.815	1.00	24.45
ATOM	1907	-	LA.	237	-5.332	51.715	-7.648	1.00	30.47
ATOM	1908	_	ALA	237	-6.424	51.484	-7.120	1.00	
MOTA	1909	_	ALA		-4.223	51.758	-6.932	1.00	21.71
MOTA	1910		GLY	238	-4.269	51.563	-5.481	1.00	19.83
ATOM	1911		GLY	238	-3.842	50.185	-5.013	1.00	17.46
ATOM	1912	-	GLY	238		49.372	-5.837	1.00	17.96
MOTA	1913	-	GLY	238	-3.387	49.844	-3.728	1.00	15.86
ATOM	1914	• .	TYR	239	-4.061	48.501	-3.275	1.00	12.97
ATOM	1915	CA	TYR	239	-3.721	48.458	-1.743	1.00	12,30
	1916	CB	TYR	239	-3.579		-1.252	1.00	11.99
ATOM	1917		TYR	239	-2.235	48.936	-0.939	1.00	12.25
MOTA	1918	CD1	TYR	239	-2.034	50.267	-0.501	1.00	12.55
MOTA		CE1	TYR	239	-0.787	50.701	-1.168	1.00	11.54
ATOM	1919	CD2	TYR	239	-1.161	48.056		1.00	11.38
ATOM	1920	CE2	TYR	239	0.072	48.470	-0.746	1.00	11.23
ATOM	1921		TYR	239	0.238	49.811	-0.426	1.00	14.40
MOTA	1922	CZ	TYR	239	1.484	50.235	-0.015	1.00	12.53
ATOM	1923	ОН	TYR	239	-4.815	47.516	-3.705		17.24
ATOM	1924	C		239	-6.007	47.800	-3.513	1.00	11.52
MOTA	1925	0	TYR	240	-4.409	46.398	-4.296	1.00	11.73
MOTA	1926	N	GLN		-5.297	45.349	-4.769	1.00	
MOTA	1927	CA	GLN	240	-5.117	45.199	-6.306	1.00	11.64
ATOM	1928	CB	GLN	240	-5.539	46.485	-7.051	1.00	14.46
ATOM	1929	CG	GLN	240		46.379	-8.546	1.00	16.63
ATOM	1930	CD	GLN	240	-5.418	45.635	-9.069	1.00	18.79
ATOM	1931	OE1	GLN	240	-4.585	47.136	-9.296	1.00	21.51
ATOM	1932	NE2	GLN	240	-6.217	44.026	-4.113	1.00	10.88
	1933	С	GLN	240	-4,935		-3.789	1.00	9.92
ATOM	1934	0	GLN	240	-3.763	43.770	-3.859	1.00	10.67
ATOM	1935	N	ASP	241		43.182	-3.230	1.00	9.82
MOTA	1936	CA	ASP	241	-5.711	41.915	-2.727	1.00	11.01
MOTA	1937	CB	ASP	241	-7.072		-1.420	1.00	12.59
MOTA		CG	ASP	241	-7.532	41.987	-1.141	1.00	15.81
ATOM	1938	OD1	ASP	241	-8.763	41.911		1.00	12.84
ATOM	1939	OD2	ASP	241	-6.719		-0.648	1.00	10.03
MOTA	1940	C	ASP	241	-5.124		-4.183	1.00	13.99
MOTA	1941		ASP	241	L -5.613	40.615	-5.276	1.00	8.45
ATOM	1942	0	ILE	242		40.170	-3.742	1.00	8.44
ATOM	1943	N	ILE	243		39.035	-4.454		8.68
MOTA	1944	CA		24		000	-4.197	1.00	10.88
MOTA	1945	CB	ILE	24			-4.760	1.00	9.70
MOTA	1946	CG2	ILE	24			-4.766	1.00	11.78
ATOM	1947	CG1	ILE	24			-4.344	1.00	8.96
ATOM	1948	CD1	ILE	24				1.00	9.65
ATOM	1949	С	ILE				- 740	1.00	9.75
ATOM	1950	0	ILE	24				1.00	
MOTA	1951	N	ALA	24				1.00	9.73
ATOM	1952	CA	ALA	24				1.00	8.94
ATOM	1953	_	ALA	24				1.00	11.10
	1954	_	ALA	24				1.00	14.74
ATOM	1955		ALA	2 '	43 -6.3		2 205	1.00	9.36
ATOM	1956		ALA	2	44 -4.9			1.00	9.36
MOTA	1957		ALA	2	44 -4.1			1.00	13.93
MOTA			ALA	_	44 -4.5	88 32.40		1.00	10.49
ATOM	1958	_	ALA	_	44 -4.2	43 31.70		1.00	13.13
MOTA	1959	•	ALA		44 -5.2			1.00	10.92
MOTA	196		ASP		45 -3.2			1.00	
MOTA	196				45 -3.1		- 0-2	1.00	
ATOM	196			_	45 -2.8		- 217	1.00	
ATOM	196				45 -2.8	392 28.66			
MOTA	196				245 -3.0		-7.996	- 01	
MOTA	196				245 -2.1		19 -6.197		
MOTA	196	_			245 -2.			1.00	, 10.40
ATOM	196	7 C	AS			=			

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ATOM	1968	0	ASP	24	15 -0.917				
ATOM	1969		ASP				-3.998	1.00	11.30
ATOM	1970						-2.905	1.00	9.06
ATOM	1971						-2.197	1.00	9.74
MOTA	1972						-0.859	1.00	11.33
ATOM	1973	OD		24			-1.011	1.00	13.92
ATOM	1974	OD:		24			0.018	1.00	15.40
ATOM	1975			24			-2.155	1.00	
ATOM	1976	C	ASP	24		25.755	-3.060	1.00	14.85
ATOM		0	ASP	24	6 -0.571		-2.544		9.71
	1977	N	THR	24	7 -1.417	25.840	-4.379	1.00	10.59
ATOM	1978	CA	THR	24		24.865		1.00	9.46
ATOM	1979	CB	THR	24		24.275	-5.261	1.00	9.37
ATOM	1980	OG1	THR	24		25.290	-6.269	1.00	11.29
ATOM	1981	CG2		24			-7.212	1.00	11.39
ATOM	1982	С	THR	24		23.800	-5.524	1.00	12.30
MOTA	1983	0	THR	241		25.442	-6.058	1.00	8.75
ATOM	1984	N	GLY	248		24.639	-6.698	1.00	11.70
ATOM	1985	CA	GLY			26.744	-6.088	1.00	8.16
ATOM	1986	C		248	- · -	27.454	-6.872	1.00	8.63
ATOM	1987	0	GLY	248		28.172	-5.992	1.00	7.49
ATOM	1988		GLY	248		28.246	-4.757	1.00	
ATOM		N	TYR	249	3.496	28.733	-6.663		10.66
ATOM	1989	CA	TYR	249	4.437	29.616	-6.005	1.00	6.67
	1990	CB	TYR	249	5.900	29.244	-6.303	1.00	6.51
ATOM	1991	CG	TYR	249	6.411	28.129		1.00	6.70
ATOM	1992	CD1	TYR	249		26.788	-5.426	1.00	6.10
ATOM	1993	CE1	TYR	249	6.786		-5.752	1.00	6.62
ATOM	1994	CD2	TYR	249	6.992	25.803	-4.929	1.00	7.14
ATOM	1995	CE2	TYR	249		28.437	-4.199	1.00	5.64
ATOM	1996	CZ	TYR	249	7.470	27.450	-3.364	1.00	5.23
ATOM	1997	ОН	TYR		7.367	26.135	-3.715	1.00	6.30
ATOM	1998	C		249	7.823	25.130	-2.903	1.00	8.55
ATOM	1999	0	TYR	249	4.202	31.046	-6.523	1.00	5.67
ATOM	2000		TYR	249	4.146	31.252	-7.740	1.00	
ATOM		N	LEU	250	4.045	31.976	-5.592	1.00	6.93
ATOM	2001	CA	LEU	250	3.894	33.381	-5.926		5.56
	2002	CB	LEU	250	3.151	34.119	-4.803	1.00	5.35
ATOM	2003	CG	LEU	250	2.830	35.587	-5.134	1.00	6.61
ATOM	2004	CD1	LEU	250	1.810	35.727		1.00	6.78
ATOM	2005	CD2	LEU	250	2.316	36.240	-6.251	1.00	7.40
ATOM	2006	С	LEU	250	5.283		-3.857	1.00	8.54
ATOM	2007	0	LEU	250	6.157	33.945	-6.147	1.00	5.86
ATOM	2008	N	ILE	251		33.797	-5.272	1.00	5.91
ATOM	2009	CA	ILE	251	5.498	34.540	-7.312	1.00	5.45
ATOM	2010	СВ	ILE	251	6.777	35.088	-7.727	1.00	6.03
ATOM	2011	CG2	ILE		7.240	34.434	-9.059	1.00	6.08
ATOM	2012	CG1		251	8.728	34.801	-9.306	1.00	7.80
ATOM	2012		ILE	251	6.975	32.941	-9.095	1.00	5.58
ATOM	2013	CD1	ILE	251	7.657	32.110	-8.038	1.00	
ATOM		C	ILE	251	6.712	36.599	-7.909	1.00	6.65
ATOM	2015	0	ILE	251	5.735	37.111	-8.484		6.10
ATOM	2016	N	ASN	252	7.760	37.291	-7.443	1.00	6.96
	2017	CA	ASN	252	7.892	38.703	-7.696	1.00	6.11
ATOM	2018	CB	ASN	252	7.145	39.615		1.00	6.61
MOTA	2019	CG	ASN	252	7.617	39.521	-6.739	1.00	7.62
ATOM	2020	OD1	ASN	252	7.166	38.626	-5.306	1.00	8.27
ATOM	2021	ND2	ASN	252	8.520	40.387	-4.587	1.00	9.37
ATOM	2022	С	ASN	252	9.377		-4.902	1.00	8.45
ATOM	2023	0	ASN	252		39.065	-7.731	1.00	6.35
ATOM	2024	N	CYS	253	10.197	38.345	-7.137	1.00	7.21
ATOM	2025	CA	CYS		9.683	40.236	-8.295	1.00	6.40
ATOM	2026	CB		253	11.048	40.768	-8.285	1.00	7.03
ATOM	2027		CYS	253	11.302	41.723	-9.464	1.00	
ATOM		SG	CYS	253	11.232	40.881	-11.077	1.00	8.85
ATOM	2028	c	CYS	253	11.309	41.552	-6.988	1.00	10.36
	2029	0	CYS	253	10.402	42.203	-6.420		7.30
ATOM	2030	N	GLY	254	12.562	41.539	-6.585	1.00	7.55
ATOM	2031	CA	GLY	254	13.063	42.360		1.00	6.67
ATOM	2032	C	GLY	254	13.850	43.536	-5.503	1.00	7.05
ATOM	2033	0	GLY	254	14.011	43.696	-6.046	1.00	7.09
ATOM	2034	N	SER	255	14.338		-7.269	1.00	7.78
ATOM	2035	CA	SER		14.942	44.380	-5.130	1.00	7.39
ATOM	2036	СВ	SER		14.942	45.634	-5.560	1.00	8.33
ATOM	2037	OG	SER			46.646	-4.420	1.00	8.09
ATOM	2038	C	SER		15.785	46.124	-3.385	1.00	9.54
ATOM	2039	0 .			16.275	45.443	-6.277	1.00	7.85
ATOM	2039	N	SER		16.710	46.348	-6.979	1.00	10.10
	2010	1.4	TYR	256	16.928	44.287	-6.184	1.00	
									7.83

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				255 1	18.151	44.106	-6.964	1.00	8.12
MOTA	2041		TYR TYR		18.966	42.909	-6.486	1.00	7.96
ATOM	2042		TYR		20.395	42.919	-7.017	1.00	7.92
ATOM	2043 2044		TYR		21.351	43.735	-6.425	1.00	9.18
MOTA MOTA	2044		TYR		22.665	43.731	-6.866	1.00	9.56
ATOM	2046		TYR		20.800	42.110	-8.068	1.00	8.38
ATOM	2047		TYR		22.119	42.114	-8.530	1.00	8.77 7.91
ATOM	2048	CZ	TYR		23.030	42.931	-7.942	1.00	10.55
ATOM	2049	OH	TYR		24.334	42.919	-8.446 -8.444	1.00	7.77
MOTA	2050	C	TYR		17.790	44.007	-9.307	1.00	9.14
MOTA	2051	0	TYR		18.510	44.559 43.310	-8.767	1.00	8.12
ATOM	2052	N	MET		16.689	43.310	-10.151	1.00	7.70
MOTA	2053	CA	MET		16.220 15.002	42.301	-10.305	1.00	8.40
ATOM	2054	CB	MET		14.582	42.102	-11.738	1.00	9.02
ATOM	2055	CG	MET MET		15.730	41.115	-12.738	1.00	9.56
ATOM	2056	SD CE	MET	257	15.233	39.485	-12.131	1.00	11.37
MOTA	2057 2058	C	MET	257	15.843	44.629	-10.670	1.00	6.94
ATOM	2059	0	MET	257	16.150	44.976	-11.819	1.00	8.48
MOTA MOTA	2060	N	ALA	258	15.189	45.427	-9.842	1.00	7.83 8.49
ATOM	2061	ÇA	ALA	258	14.807	46.786	-10.242	1.00 1.00	8.60
ATOM	2062	CB	ALA	258	13.940	47.433	-9.204	1.00	8.95
ATOM	2063	C	ALA	258	16.074	47.582	-10.550 -11.526	1.00	10.68
ATOM	2064	0	ALA	258	16.128	48.339	-9.717	1.00	9.55
ATOM	2065	N	HIS	259	17.075	47.456	-9.987	1.00	9.84
ATOM	2066	CA	HIS	259	18.325	48.184 47.968	-8.806	1.00	10.82
ATOM	2067	CB	HIS	259	19.298 20.581	48.672	-8.960	1.00	12.01
MOTA	2068	CG	HIS	259 259	20.381	50.004	-8.919	1.00	11.84
MOTA	2069	CD2	HIS HIS	259	21.801	48.079	-9.209	1.00	14.52
MOTA	2070	ND1 CE1	HIS	259	22.701	49.050	-9.270	1.00	12.90
MOTA	2071	NE2	HIS	259	22.106	50.209	-9.115	1.00	14.66
ATOM	2072 2073	C	HIS	259	18.949	47.746	-11.296	1.00	9.17
ATOM	2074	0	HIS	259	19.275	48.580	-12.144	1.00	11.20
ATOM ATOM	2075	N	LEU	260	19.091	46.450	-11.529	1.00	9.71 11.16
ATOM	2076	CA	LEU	260	19.763	45.917	-12.699	1.00 1.00	13.64
ATOM	2077	CB	LEU	260	19.771	44.362	-12.647	1.00	14.53
MOTA	2078	CG	LEU	260	20.621	43.697	-11.579 -11.659	1.00	15.33
MOTA	2079	CD1	LEU	260	20.446	42.195	-11.700	1.00	18.49
MOTA	2080	CD2	LEU	260	22.081	44.131 46.315	-13.989	1.00	10.90
ATOM	2081	C	LEU	260	19.044 19.715	46.435	-15.017	1.00	11.94
MOTA	2082	0	LEU	260 261	17.723	46.442	-13.932	1.00	9.82
MOTA	2083	N	THR THR	261	16.920	46.680	-15.141	1.00	10.23
ATOM	2084	CA CB	THR	261	15.671	45.798	-15.202	1.00	9.32
ATOM	2085 2086	OG1	THR	261	14.737	46.138	-14.174	1.00	9.59
ATOM	2086	CG2	THR	261	16.000	44.325	-15.098	1.00	10.96
ATOM ATOM	2088	C	THR	261	16.492	48.151	-15.298	1.00	10.83 12.22
ATOM	2089	0	THR	261	15.664	48.493	-16.138	1.00 1.00	12.22
ATOM	2090	N	ASN	262	17.009	48.999	-14.417	1.00	13.99
ATOM	2091	CA	ASN	262	16.643	50.411	-14.405 -15.670	1.00	16.72
MOTA	2092	CB	ASN	262	17.162	51.124	-15.414	1.00	18.91
MOTA	2093	CG	ASN	262	17.122	52.624 53.032	-14.306	1.00	23.20
MOTA	2094	OD1	ASN	262	17.484 16.604	53.423	-16.351	1.00	23.32
MOTA	2095	ND2	ASN	262 262	15.143	50.639	-14.281	1.00	14.56
MOTA	2096	C	ASN	262	14.524	51.455	-14.945	1.00	17.11
MOTA	2097	0	asn asn	263	14.570	49.836	-13.381	1.00	13.82
ATOM	2098	N CA	ASN	263	13.148	49.902	-13.081	1.00	15.46
ATOM	2099 2100	CB	ASN	263	12.863	51.289	-12.502	1.00	17.97
ATOM	2100	CG	ASN	263	12.214	51.276	-11.157	1.00	17.06
ATOM ATOM	2102	OD1	ASN	263	12.128	50.271	-10.466	1.00	15.00 25.64
ATOM	2103	ND2	ASN	263	11.533	52.359	-10.866	1.00	13.77
ATOM	2104	С	ASN	263		49.450	-14.215	1.00 1.00	18.41
ATOM	2105	0	ASN	263		49.566	-14.160 -15.236	1.00	13.79
ATOM	2106	N	TYR	264		48.764	-16.255	1.00	14.19
MOTA	2107	CA	TYR	264		48.149	-17.416	1.00	15.13
ATOM	2108	CB	TYR	264		47.613 46.818	-18.494	1.00	16.36
MOTA	2109	CG	TYR	264		47.371	-19.362	1.00	17.78
ATOM	2110	CD1		264	_	46.634	-20.350	1.00	18.06
MOTA	2111	CE1		264 264		45.484	-18.745	1.00	16.68
ATOM	2112	CD2		264		44.748	-19.760	1.00	16.65
MOTA	2113	CE2							

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ATOM	2114	CZ	TYR	264	10.716	45.314	-20.586	1.00	18.96
ATOM	2115	ОН	TYR	264	10.037	44.587	-21.573	1.00	18.75
ATOM ATOM	2116	C	TYR	264	11.078	47.051	-15.593	1.00	12.40
ATOM	2117 2118	N	TYR	264	9.880	46.958	-15.851	1.00	13.61
ATOM	2119	CA	TYR TYR	265 265	11.724	46.245	-14.738	1.00	10.62
ATOM	2120	CB	TYR	265	11.038 11.580	45.308	-13.845	1.00	9.32
ATOM	2121	CG	TYR	265	11.384	43.896 43.145	-13.877	1.00	9.65
ATOM	2122	CD1		265	11.979	41.897	-15.197 -15.374	1.00	9.18
ATOM	2123	CE1		265	11.788	41.151	-16.513	1.00 1.00	9.12
ATOM	2124	CD2	TYR	265	10.575	43.607	-16.232	1.00	9.35 9.97
ATOM	2125	CE2		265	10.412	42.861	-17.391	1.00	9.60
ATOM ATOM	2126	CZ	TYR	265	11.019	41.653	-17.546	1.00	8.98
ATOM	2127	ОН	TYR	265	10.956	40.929	-18.694	1.00	9.24
ATOM	2128 2129	C O	TYR TYR	265	11.143	45.898	-12.455	1.00	8.87
ATOM	2130	Ŋ	LYS	265 266	12.165	45.736	-11.793	1.00	10.25
ATOM	2131	CA	LYS	266	10.091 10.042	46.591	-12.039	1.00	9.35
ATOM	2132	CB	LYS	266	8.764	47.206 48.067	-10.722	1.00	10.27
MOTA	2133	CG	LYS	266	8.798	49.269	-10.642 -11.544	1.00	11.78
ATOM	2134	CD	LYS	266	7.679	50.219	-11.609	1.00	15.74
ATOM	2135	CE	LYS	266	8.060	51.436	-12.461	1.00	20.41 27.15
ATOM	2136	NZ	LYS	266	8.880	51.073	-13.684	1.00	38.27
ATOM	2137	C	LYS	266	9.917	46.141	-9.642	1.00	9.64
ATOM	2138	0	LYS	266	9.483	45.006	-9.859	1.00	11.33
ATOM ATOM	2139	N	ALA	267	10.398	46.485	-8.457	1.00	8.21
ATOM	2140 2141	CA	ALA	267	10.177	45.669	-7.302	1.00	8.00
ATOM	2142	CB C	ALA ALA	267	11.263	45.935	-6.279	1.00	9.27
ATOM	2143	0	ALA	267 267	8.810	46.112	-6.747	1.00	8.06
ATOM	2144	N	PRO	268	8.703 7.786	47.252	-6.265	1.00	9.31
ATOM	2145	CD	PRO	268	7.704	45.314 43.960	-6.903 -7.464	1.00	7.87
ATOM	2146	CA	PRO	268	6.464	45.815	-6.507	1.00 1.00	8.45
MOTA	2147	CB	PRO	268	5.497	44.732	-6.971	1.00	8.53 8.95
ATOM	2148	CG	PRO	268	6.340	43.491	-6.981	1.00	9.67
ATOM	2149	С	PRO	268	6.342	46.060	-5.020	1.00	7.51
ATOM	2150	0	PRO	268	6.832	45.247	-4.237	1.00	8.65
ATOM ATOM	2151	N	ILE	269	5.648	47.157	-4.658	1.00	7.63
ATOM	2152 2153	CA	ILE	269	5.356	47.441	~3.254	1.00	7.94
ATOM	2154	CB CG2	ILE ILE	269 269	5.120	48.928	-2.981	1.00	9.79
ATOM	2155	CG1	ILE	269	4.494 6.437	49.172	-1.634	1.00	10.56
ATOM	2156	CD1	ILE	269	6.187	49.720 - 51.182	-3.185	1.00	13.68
ATOM	2157	С	ILE	269	4.170	46.593	-3.479 -2.837	1.00	23.32
ATOM	2158	0	ILE	269	3.149	46.540	-3.511	1.00	7.83
ATOM	2 1 59	N	HIS	270	4.317	45.894	-1.703	1.00	9.16 7.29
ATOM	2160	CA	HIS	270	3.276	45.019	-1.206	1.00	7.01
ATOM	2161	CB	HIS	270	3.400	43.626	-1.835	1.00	7.25
ATOM ATOM	2162	CG	HIS	270	4.744	43.024	-1.598	1.00	7.13
ATOM	2163 2164	CD2 ND1	HIS	270	5.128	42.038	-0.746	1.00	7.31
ATOM	2165	CE1	HIS HIS	270 270	5.880	43.389	-2.273	1.00	7.07
ATOM	2166	NE2	HIS	270	6.904 6.489	42.683 41.831	-1.826	1.00	7.87
ATOM	2167	C	HIS	270	3.274	44.991	-0.890 0.302	1.00	7.31
ATOM	2168	0	HIS	270	4.212	45.458	0.936	1.00 1.00	6.54
MOTA	2169	N	ARG	271	2.201	44.490	0.896	1.00	7.63 6.78
ATOM	2170	CA	ARG	271	1.988	44.467	2.318	1.00	6.60
ATOM	2171	CB	ARG	271	1.366	45.769	2.853	1.00	7.26
ATOM	2172	CG	ARG	271	-0.088	45.972	2.398	1.00	8.12
ATOM ATOM	2173	CD	ARG	271	-0.543	47.381	2.652	1.00	8.48
ATOM	2174 2175	NE CZ	ARG	271	-1.974	47.504	2.297	1.00	9.27
ATOM	2176	NH1	ARG ARG	271	-2.643	48.651	2.312	1.00	9.64
ATOM	2177	NH2	ARG	271 271	-2.060 -3.930	49.802	2.648	1.00	10.45
ATOM	2178	C	ARG	271	1.144	48.660 43.252	1.968	1.00	11.63
ATOM	2179	ō	ARG	271	0.517	42.637	2.682 1.805	1.00	6.79
ATOM	2180	N	VAL	272	1.154	42.887	3.953	1.00 1.00	7.95
ATOM	2181	CA	VAL	272	0.444	41.736	4.493	1.00	7.39 6.97
ATOM	2182	CB	VAL	272	1.369	40.830	5.328	1.00	6.97 7.37
ATOM	2183	CG1	VAL	272	0.615	39.661	5.865	1.00	9.31
ATOM	2184	CG2	VAL	272	2.609	40.388	4.562	1.00	9.68
ATOM	2185	C	VAL	272	-0.712	42.173	5.378	1.00	6.78
ATOM	2186	0	VAL	272	-0.470	42.805	6.415	1.00	7.67

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						- 109 -				7.33
			* VC	273	-1.93	17	11.839	4.950	1.00 1.00	8.38
MOTA	2187	N	LYS	273	-3.0	51 -	12.135	5.792	1.00	9.72
ATOM	2188	CA	LYS LYS	273	-4.3	64 '	41.763	5.047	1.00	13.66
ATOM	2189	CB CG	LYS	273	-4.6	58	42.765	3.950 3.437	1.00	20.08
MOTA	2190	CD	LYS	273	-6.0	90	42.725	2.873	1.00	21.66
MOTA	2191	CE	LYS	273	-6.3	81	41.379	2.413	1.00	19.22
ATOM	2192	NZ	LYS	273	-7.B		41.227	7.047	1.00	7.72
MOTA	2193	C	LYS	273	-3.0	•	41.256	7.023	1.00	8.06
ATOM	2194 2195	0	LYS	273	-2.6		40.112	8.114	1.00	7.85
ATOM	2196	N	TRP	274	-3.6		41.812 41.041	9.322	1.00	8.01
ATOM	2197	CA	TRP	274	-3.9		41.953	10.481	1.00	8.38
ATOM	2198	СВ	TRP	274	-4.		41.210	11.655	1.00	8.22
ATOM ATOM	2199	CG	TRP	274	-4.		41.225	12.078	1.00	8.59
ATOM	2200	CD2	TRP	274	-6.: -6.		40.370	13.188	1.00	9.28 10.81
ATOM	2201	CE2	TRP	274	-7.		41.859	11.630	1.00	8.98
ATOM	2202	CE3	TRP	274 274	-4.		40.377	12.490	1.00 1.00	9.16
ATOM	2203	CD1	TRP	274		074	39.850	13.430	1.00	9.84
MOTA	2204	NEI	TRP TRP	274		485	40.145	13.881	1.00	12.76
ATOM	2205	CZ2	TRP	274	-8.	570	41.630	12.309 13.403	1.00	12.58
MOTA	2206	CZ3 CH2	TRP	274	- R .	591	40.765	9.043	1.00	7.32
MOTA	2207	CHZ	TRP	274	- 5 .	114	40.123	8.598	1.00	8.37
MOTA	2208	0	TRP	274	-6	. 156	40.621	9.345	1.00	7.40
MOTA	2209	N	VAL	275		.963	38.854	9.221	1.00	7.99
MOTA	2210 2211	CA	VAL	275		.042	37.883 37.057	7.931	1.00	11.04
ATOM	2212	CB	VAL	275		.913	36.169	7.828	1.00	13.41
ATOM	2213	CG1	VAL	275		.152	37.904	6.702	1.00	15.17
MOTA MOTA	2214	CG2	VAL	279		.765	37.000	10.457	1.00	7.32
ATOM	2215	C	VAL	279		.933	36.547	10.759	1.00	8.66 7.50
ATOM	2216	0	VAL	27		.818	36.774	11.175	1.00	8.58
ATOM	2217	N	ASN	27		.930	35.898	12.365	1.00	9.69
ATOM	2218	CA	ASN	27 27		7.921	36.377	13.414	1.00	10.43
MOTA	2219	CB	ASN	27		7.600	35.733	14.757	1.00	9.69
ATOM	2220	CG	ASN	27	_	5.631	34.956	14.885	1.00	12.06
ATOM	2221	OD I	_	27	-	8.414	35.995	15.765	1.00	8.56
ATOM	2222	ND:	ASN	27		7.172	34.443	11.976 12.021	1.00	9.02
MOTA	2223	с 0	ASN	27		8.281	33.914	11.504	1.00	8.26
MOTA	2224	И	ALA	2	77 -	6.107	33.815	10.982	1.00	8.04
MOTA	2225	CA		2.	7 7 -	6.107	32.466	9.514	1.00	9.72
ATOM	2226	CB	ALA	2		6.438	32.469	11.136	1.00	7.91
MOTA	2227 2228	C	ALA			4.711	31.860 32.537	10.998	1.00	8.82
MOTA	2229	0	ALA			3.705	30.592	11.445	1.00	7.51
MOTA MOTA	2230	N	GLU			4.674	29.801	11.557	1.00	7.98
ATOM	2231			_		-3.460	28.504	12.302	1.00	10.38 11.75
ATOM	2232	CE		_		-3.727 -2.539	27.650	12.655	1.00	10.88
ATOM	2233	~ .		_		-1.613	28.347	13.638	1.00	12.63
MOTA	2234					-0.419	28.424	13.314	1.00 1.00	10.57
ATOM	2235		E1 GL		278	-2.074	28.833	14.680	1.00	8.98
MOTA	2236	_	E2 GL		278	-3.034	29.524	10.111	1.00	12.15
MOTA	223	_		-	278	-3.719	28.836	9.346 9.738	1.00	8.14
MOTA	223				279	-1.864	30.037		1.00	8.39
MOTA	223	_	A AR		279	-1.410		- 470	1.00	10.37
MOTA	224 224	٠.	B AR		279	-2.095		- 010	1.00	10.01
MOTA	224		G AR	.G	279	-1.659			1.00	9.69
MOTA	224		D AF	kG	279	-2.541			1.00	
ATOM	224		NE AF	₹G	279	-2.026		6.775	1.00	
MOTA MOTA	224		CZ AI		279	-0.965 -0.368			1.00	
ATOM	224			RG	279	-0.490			1.00	
ATOM	224			RG	279	0.09		0 8.275		
ATOM	224	48	•	RG	279 279	0.82		9.252		•
MOTA	22		_	RG	280	0.59		1 7.095	- ^	•
MOTA	22		• •	LN	280	2.00	6 29.50	6.778		
ATOM		51		LN	280	2.31	.g 28.08			
ATOM	22	52		LN	280	2.04	3 27.04	~ 77		0 8.58
ATOM	22	53		LN SLN	280	2.18	8 25.64			
MOTA		254	~-	3LN	280	2.06				0 8.97
ATOM		255		GLN	280	2.5				0 6.21
MOTA	٠	256		GLN	280	2.3				7.53
ATOM	•	257 258		GLN	280			- 77		00 6.11
MOTA	•	258 259		SER	281	3.5	54 31.0			
OTA	r, 2									

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ATOM	226	50 C.	A SE	P n	0.7				
ATOM	226	-			81 4.1	00.		3 00	_
ATOM	226				81 4.0		5.109	1.00	
ATOM	226	-			81 4.5	20 34.121		1.00	
ATOM	226	_	SE		81 5.63			1.00	0.04
ATOM			SEF	₹ 2.	81 6.37			1.00	6.56
	226		LEC	J 2:	82 5.95			1.00	
ATOM	226	6 C2	LEU		32 7.24	. •		1.00	
ATOM	226	7 CE					3.352	1.00	9.10
ATOM	2268					~~.505	3.195	1.00	6.03
ATOM	2269						4.203		6.16
ATOM	2270					1 26.441	3.942	1.00	7.21
ATOM					2 6.34	0 28.188		1.00	8.79
ATOM	2273	_	LEU	28	2 8.02		5.661	1.00	8.29
	2272	_	LEU	28			2.173	1.00	5.52
ATOM	2273		PRO	28			1.071	1.00	5.66
ATOM	2274	CD	PRO	28			2.318	1.00	
ATOM	2275	CA	PRO	28			3.463	1.00	5.55
ATOM	2276		PRO				1.222	1.00	5.92
ATOM	2277			28.		33.815	1.631		5.72
ATOM	2278		PRO	283	9.624		3.131	1.00	6.44
ATOM		C	PRO	28:	3 10.795			1.00	6.28
ATOM	2279	0	PRO	283			1.057	1.00	4.97
	2280	N	PHE	284			2.006	1.00	5.92
ATOM	2281	CA	PHE	284		,20	-0.187	1.00	5.22
ATOM	2282	CB	PHE	284			-0.602	1.00	
ATOM	2283	CG	PHE			30.323	-1.566	1.00	4.80
ATOM	2284	CD1		284		29.960	-1.983		5.14
ATOM	2285			284	15.089	29.473	-1.057	1.00	4.79
ATOM		CD2	PHE	284	14.591	30.026		1.00	5.39
	2286	CE1	PHE	284		29.032	-3.286	1.00	5.88
ATOM	2287	CE2	PHE	284			-1.451	1.00	5.76
ATOM	2288	CZ	PHE	284		29.633	-3.714	1.00	5.70
ATOM	2289	С	PHE		16.714	29.109	-2.787	1.00	
ATOM	2290	0	PHE	284	13.119	32.795	-1.263		5.57
ATOM	2291	N		284	12.566	33.190	-2.308	1.00	4.78
ATOM	2292		PHE	285	14.114	33.448	-0.659	1.00	5.98
ATOM		CA	PHE	285	14.656	34.687		1.00	5.01
ATOM	2293	CB	PHE	285	15.058	35.637	-1.215	1.00	5.10
	2294	CG	PHE	285	13.858	35.037	-0.062	1.00	6.13
ATOM	2295	CD1	PHE	285	13.665	36.096	0.747	1.00	6.38
ATOM	2296	CD2	PHE	285		35.656	2.044	1.00	6.54
ATOM	2297	CE1	PHE		12.909	36.933	0.195	1.00	
ATOM	2298	CE2	PHE	285	12.534	36.014	2.765	1.00	6.45
ATOM	2299	CZ		285	11.781	37.303	0.891		7.21
ATOM	2300		PHE	285	11.610	36.853	2.177	1.00	7.45
ATOM		C	PHE	285	15.812	34.333		1.00	7.71
ATOM	2301	0	PHE	285	16.815	33.800	-2.108	1.00	5.08
	2302	N	VAL	286	15.658		-1.608	1.00	6.02
ATOM	2303	CA	VAL	286	16.696	34.588	-3.399	1.00	5.58
ATOM	2304	CB	VAL	286		34.255	-4.364	1.00	5.56
ATOM	2305	CG1	LAV	286	16.104	34.056	-5.766	1.00	
ATOM	2306	CG2	VAL		17.189	33.783	-6.814	1.00	5.78
ATOM	2307	C		286	15.065	32.922	-5.710		7.42
ATOM	2308		VAL	286	17.756	35.372	-4.347	1.00	7.19
ATOM	2309	0	VAL	286	17.569	36.453	-4.895	1.00	5.98
ATOM		N	ASN	287	18.839	35.082	7.095	1.00	6.92
ATOM	2310	CA	ASN	287	20.008	35.922	-3.642	1.00	5.82
	2311	CB	ASN	287	20.324	36.042	-3.466	1.00	6.12
ATOM	2312	CG	ASN	287	19.235		-1.971	1.00	6.40
ATOM	2313	OD1	ASN	287	18.623	36.737	-1.183	1.00	6.67
ATOM	2314	ND2	ASN			37.682	-1.683	1.00	
ATOM	2315	C	ASN	207	19.036	36.262	0.073	1.00	7.35
ATOM	2316	ō		287	21.187	35.296	-4.216		6.70
ATOM	2317		ASN	287	21.271	34.072	-4.300	1.00	5.72
ATOM		N	LEU	288	22.049	36.145		1.00	6.46
ATOM	2318		LEU		23.223	35.679	-4.781	1.00	6.71
	2319	CB	LEU		23.538	35.679	-5.499	1.00	6.46
ATOM	2320	CG	LEU		22.371	36.703	-6.595	1.00	7.57
ATOM	2321	CD1	LEU		22.819	36.977	-7.570	1.00	8.20
ATOM	2322		LEU			37.998	-8.621	1.00	0.20
ATOM	2323		LEU		21.880	35.687	-8.189		10.08
ATOM	2324				24.381	35.444	-4.525	1.00	8.32
ATOM	2325		LEU		24.140	35.277	-3.317	1.00	7.33
ATOM			GLY		25.607	35.358		1.00	8.58
	2326		3LY		6.765	35.216	-5.037	1.00	7.93
ATOM	2327	C (GLY		7.242		-4.155	1.00	7.86
MOTA	2328				6.890	36.571	-3.667	1.00	7.24
ATOM	2329				0.090	37.634	-4.186	1.00	
ATOM	2330				8.075	36.559	-2.633	1.00	8.44
ATOM	2331	_			8.503	37.789	-1.986		7.71
ATOM		_			9.407	37.453	-0.813	1.00	8.91
	-332	CG I	YR :		9.638	38.614	0.135	1.00	9.56
							0.172	1.00	9.12

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ATOM	2333	CD1	TYR	290	28.720	38.961	1.118	1.00	10.55
ATOM	2334	CEl	TYR	290	28.949	40.041	1.966	1.00	12.13
ATOM	2335	CD2	TYR	290	30.792	39.367	0.036	1.00	12.09
MOTA	2336	CE3	TYR	290	31.035	40.426	0.887 1.861	1.00	13.43 13.85
MOTA	2337	CZ	TYR	290	30.129 30.407	40.766 41.847	2.679	1.00	16.61
ATOM	2338	OH	TYR TYR	290 290	29.196	38.783	-2.903	1.00	8.98
ATOM	2339 2340	0	TYR	290	28.979	39.980	-2.814	1.00	9.66
MOTA MOTA	2341	N	ASP	291	30.009	38.246	-3.816	1.00	9.63
ATOM	2342	CA	ASP	291	30.738	39.081	-4.766	1.00	11.13
MOTA	2343	CB	ASP	291	32.143	38.545	-4.920	1.00	14.78
ATOM	2344	CG	ASP	291	33.015	38.830	-3.715	1.00	19.43
MOTA	2345	OD1	ASP	291	34.005	38.109	-3.515 -2.963	1.00	30.38 21.52
ATOM	2346	OD2	ASP	291	32.776	39.787	-6.123	1.00 1.00	10.76
MOTA	2347	C	ASP ASP	291 291	30.075 30.676	39.198 39.770	-7.035	1.00	14.21
ATOM	2348 2349	O N	SER	292	28.867	38.636	-6.294	1.00	10.05
ATOM ATOM	2350	CA	SER	292	28.226	38.714	-7.606	1.00	9.39
ATOM	2351	CB	SER	292	26.908	37.921	-7.562	1.00	9.60
ATOM	2352	OG	SER	292	27.117	36.538	-7.241	1.00	10.02
MOTA	2353	Ĉ	SER	292	27.915	40.181	-7.922	1.00	9.65
ATOM	2354	0	SER	292	27.303	40.934	-7.170	1.00 1.00	10.11 11.44
ATOM	2355	N	VAL	293	28.284	40.587	-9.123 -9.675	1.00	12.30
ATOM	2356	CA	VAL	293 293	27.948 29.177	41.879 42.809	-9.749	1.00	14.95
MOTA	2357	CB CG1	VAL VAL	293	28.691	44.199	-10.166	1.00	20.38
ATOM ATOM	2358 2359	CG2	VAL	293	29.947	42.902	-8.464	1.00	18.62
ATOM	2360	C	VAL	293	27.402	41.683	-11.091	1.00	13.15
ATOM	2361	0	VAL	293	27.976	41.020	-11.971	1.00	17.31
ATOM	2362	N	ILE	294	26.232	42.246	-11.309	1.00	13.36
MOTA	2363	CA	ILE	294	25.669	42.289	-12.650	1.00	16.26 18.21
ATOM	2364	CB	ILE	294	24.283	41.645	-12.648 -13.941	1.00	22.79
ATOM	2365	CG2	ILE	294 294	23.540 24.529	41.879 40.135	-12.350	1.00	19.50
MOTA	2366 2367	CG1 CD1	ILE	294	23.255	39.371	-12.397	1.00	21.00
MOTA MOTA	2368	C	ILE	294	25.616	43.756	-13.059	1.00	14.95
ATOM	2369	ō	ILE	294	25.193	44.619	-12.311	1.00	14.96
ATOM	2370	N	ASP	295	26.164	44.020	-14.235	1.00	15.39
ATOM	2371	CA	ASP	295	26.203	45.398	-14.709	1.00	16.58 23.82
ATOM	2372	CB	ASP	295	27.214	45.501	-15.857 -15.298	1.00	30.17
ATOM	2373	CG	ASP	295	28.612 29.304	45.188 44.457	-16.044	1.00	42.83
ATOM	2374	OD1 OD2	ASP ASP	295 295	29.000	45.638	-14.184	1.00	32.91
ATOM ATOM	2375 2376	C C	ASP	295	24.803	45.841	-15.109	1.00	13.64
ATOM	2377	Ö	ASP	295	24.072	45.199	-15.856	1.00	14.07
ATOM	2378	N	PRO	296	24.390	46.969	-14.533	1.00	12.78
ATOM	2379	CD	PRO	296	25.049	47.684	-13.426	1.00	14.44
MOTA	2380	CA	PRO	296	23.029	47.467	-14.847	1.00	12.67 14.23
ATOM	2381	CB	PRO	296	22.877	48.659	-13.923 -12.818	1.00	16.25
MOTA	2382	CG	PRO PRO	296 296	23.840 22.825	48.351 47.803	-16.319	1.00	12.63
ATOM ATOM	2383 2384	c o	PRO	296	23.750	48.221	-17.032	1.00	14.48
ATOM	2385	N	PHE	297	21.602	47.615	-16.800	1.00	11.48
ATOM	2386	CA	PHE	297	21.260	47.872	-18.195	1.00	11.96
ATOM	2387	CB	PHE	297	21.388	46.632	-19.046	1.00	12.04
ATOM	2388	CG	PHE	297	20.543	45.425	-18.690	1.00	12.30
MOTA	2389	CD1	PHE	297	19.390	45.126	-19.386 -17.664	1.00 1.00	15.33 12.58
MOTA	2390	CD2	PHE	297	20.900	44.597 44.005	-17.664	1.00	17.14
MOTA	2391	CE1	PHE	297 297	18.648 20.121	43.510	-17.311	1.00	14.52
ATOM	2392	CZ CE2.	PHE	297	18.969	43.235	-18.003	1.00	16.56
MOTA MOTA	2393 2394	C	PHE	297	19.837	48.421	-18.246	1.00	13.07
MOTA	2395	0	PHE	297	19.162	48.472	-17.219	1.00	14.15
ATOM	2396	N	ASP	298	19.390	48.809	-19.429	1.00	16.06
ATOM	2397	CA	ASP	298	18.024	49.272	-19.601	1.00	15.45
ATOM	2398	CB	ASP	298	18.023	50.788	-19.547	1.00	17.44 17.86
MOTA	2399	CG	ASP	298	16.619	51.374	-19.488 -19.809	1.00 1.00	17.50
ATOM	2400	OD1	ASP	298 298	15.634 16.580	50.717 52.580	-19.143	1.00	20.86
ATOM	2401	OD2 C	ASP ASP	298	17.436	48.753	-20.900	1.00	16.52
ATOM ATOM	2402 2403	0	ASP	298	17.736	49.281	-21.973	1.00	17.05
ATOM	2403	Ŋ	PRO	299	16.541	47.776	-20.829	1.00	16.19
ATOM	2405	CD	PRO	299	16.199	47.050	-19.589	1.00	17.38

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MOTA	2406	CA	PRO	299	15.887	47.212	-22.014	1.00	16.63
ATOM	2407	CB	PRO	299	15.397	45.853	-21.561	1.00	19.69
ATOM	2408	CG	PRO	299	15.676	45.745	-20.112	1.00	21.06
ATOM	2409	C	PRO	299	14.854	48.081	-22.726	1.00	17.45
ATOM	2410	0	PRO	299	14.213	47.662	-23.730	1.00	18.54
ATOM	2411	И	ARG	300	14.703	49.327	-22.232	1.00	16.34
ATOM	2412	CA	ARG	300	13.857	50.321	-22.881	1.00	18.12
ATOM	2413	CB	ARG	300	13.086	51.146	-21.833	1.00	19.33
ATOM	2414	CG	ARG	300	11.959	50.301	-21.242	1.00	21.93
ATOM	2415	CD	ARG	300	11.237	50.861	-20.020	1.00	25.26
ATOM	2416	NE	ARG	300	12.231	51.198	-19.046	1.00	30.85
ATOM	2417	CZ	ARG	300	12.419	51.701	-17.857	1.00	29.50
ATOM	2418	NH1	ARG	300	11.422	52.069	-17.096	1.00	32.95
ATOM	2419	NH2	ARG	300	13.671	51.781	-17.407	1.00	30.69
ATOM	2420	С	ARG	300	14.691	51.279	-23.726	1.00	17.96
ATOM	2421	0	ARG	300	14.138	52.081	-24.462	1.00	17.01
ATOM	2422	N	GLU	301	15.997	51.254	-23.552	1.00	17.71
ATOM	2423	CA	GLU	301	16.913	52.185	-24.206	1.00	19.38
ATOM	2424	С	GLU	301	17.619	51.524	-25.392	1.00	18.52
ATOM	2425	0	GLU	301	18.127	50.400	-25.261	1.00	17.52
ATOM	2426	CB	GLU	301	17.949	52.595	-23.157	1.00	23.66
ATOM	2427	CG	GLU	301	17.521	53.757	-22.322	1.00	27.35
ATOM	2428	CD	GLU	301	16.969	54.959	-23.059	1.00	32.53
ATOM	2429	OE1	GLU	301	17.705	55.499	-23.901	1.00	38.75
ATOM	2430	OE2	GLU	301	15.841	55.411	-22.764	1.00	38.29
ATOM	2431	N	PRO	302	17.667	52.160	-26.553	1.00	18.63
ATOM	2432	CD	PRO	302	17.042	53.464	-26.839	1.00	21.36
ATOM	2433	CA	PRO	302	18.277	51.571	-27.738	1.00	20.96
ATOM	2434	CB	PRO	302	18.222	52.693	-28.776	1.00	22.61
ATOM	2435	CG	PRO	302	17.001	53.446	-28.341	1.00	22.90
ATOM	2436	C	PRO	302	19.683	51.057	-27.579	1.00	21.62
ATOM ATOM	2437	0	PRO	302	19.874	49.926	-28.009	1.00	24.93
ATOM	2438	N	ASN	303	20.520	51.712	-26.771	1.00	21.61
ATOM	2439 2440	CA CB	ASN	303	21.840	51.125	-26.582	1.00	22.90
ATOM	2441	CG	ASN ASN	303 303	22.905	52.194	-26.448	1.00	26.88
ATOM	2441	OD1	ASN	303	22.642	53.204	-25.353	1.00	27.57
ATOM	2442	ND2	ASN	303	21.822 23.353	52.996 54.329	-24.467	1.00	23.80
ATOM	2444	C	ASN	303	21.931	50.221	-25.453	1.00	29.21
ATOM	2445	0	ASN	303	23.039	49.773	-25.360 -25.049	1.00	20.67
ATOM	2446	N	GLY	304	20.847	49.989	-24.661	1.00 1.00	23.78
ATOM	2447	CA	GLY	304	20.793	49.190	-23.443	1.00	17.93
ATOM	2448	C	GLY	304	21.488	49.856	-22.276	1.00	18.03 17.52
ATOM	2449	ō	GLY	304	21.576	49.239	-21.215	1.00	20.50
ATOM	2450	N	LYS	305	22.009	51.071	-22.342	1.00	18.09
ATOM	2451	CA	LYS	305	22.768	51.590	-21.208	1.00	20.79
ATOM	2452	C	LYS	305	21.921	52.252	-20.147	1.00	20.79
ATOM	2453	0	LYS	305	20.850	52.777	-20.392	1.00	21.26
ATOM	2454	CB	LYS	305	23.884	52.524	-21.675	1.00	24.72
ATOM	2455	CG	LYS	305	25.002	51.789	-22.421	1.00	30.61
ATOM	2456	CD	LYS	305	26.032	52.816	-22.869	1.00	36.33
ATOM	2457	CE	LYS	305	26.246	52.908	-24.360	1.00	39.54
ATOM	2458	NZ	LYS	305	27.649	52.574	-24.760	1.00	51.21
ATOM	2459	N	SER	306	22.461	52.202	-18.921	1.00	18.96
ATOM	2460	CA	SER	306	21.758	52.837	-17.816	1.00	19.30
ATOM	2461	CB	SER	306	21.210	51.732	-16.911	1.00	23.77
ATOM	2462	`OG	SER	306	21.758	51.769	-15.640	1.00	26.38
ATOM	2463	С	SER	306	22.711	53.732	-17.050	1.00	16.95
ATOM	2464	0	SER	306	23.919	53.528	-16.996	1.00	20.29
ATOM	2465	Ν .	ASP	307	22. 1 59	54.728	-16.365	1.00	18.07
ATOM	2466	CA	ASP	307	22.902	55.647	-15.527	1.00	17.75
MOTA	2467	CB	ASP	307	22.343	57.066	-15.646	1.00	19.69
ATOM	2468	CG	ASP	307	22.554	57.644	-17.030	1.00	21.31
ATOM	2469	OD1	ASP	307	23.544	57.289	-17.717	1.00	25.76
ATOM	2470	OD2	ASP	307	21.697	58.413	-17.492	1.00	22.42
ATOM	2471	C	ASP	307	23.003	55.194	-14.083	1.00	17.12
ATOM	2472	0	ASP	307	23.267	55.998	-13.150	1.00	15.97
ATOM	2473	N	ARG	308	22.897	53.886	-13.877	1.00	18.84
ATOM	2474	CA	ARG	308	23.109	53.313	-12.542	1.00	17.51
ATOM	2475	CB	ARG	308	22.067	52.271	-12.242	1.00	16.86
ATOM	2476	CG	ARG	308	20.688	52.745	-11.848	1.00	15.69
ATOM	2477	CD	ARG	308	19.627	51.694	-11.982	1.00	18.04
ATOM	2478	NE	ARG	308	18.312	52.224	-11.687	1.00	17.41

ATOM 2479 CZ ARG 308 17.733 52.219 -10.497 1.00 15.39 ATOM 2480 NH1 ARG 308 19.288 51.740 -9.404 1.00 14.58 ATOM 2481 NH2 ARG 308 16.517 52.713 -10.426 1.00 19.03 ATOM 2482 C ARG 308 24.511 52.680 -12.443 1.00 18.59 ATOM 2483 O ARG 308 25.055 52.218 -13.440 1.00 25.55 ATOM 2484 N GLU 309 25.070 52.659 -11.241 1.00 18.16 ATOM 2485 CA GLU 309 26.350 52.054 -10.946 1.00 19.38 ATOM 2486 CB GLU 309 27.058 52.935 -9.907 1.00 21.98 ATOM 2487 CG GLU 309 27.442 54.299 -10.501 1.00 35.52 ATOM 2488 CD GLU 309 28.319 54.244 -11.731 1.00 30.05 ATOM 2489 OE1 GLU 309 28.319 54.244 -11.731 1.00 36.16 ATOM 2489 OE2 GLU 309 28.114 55.058 -12.663 1.00 37.66 ATOM 2490 OE2 GLU 309 26.233 50.607 -10.484 1.00 15.87 ATOM 2491 C GLU 309 26.233 50.607 -10.484 1.00 15.87 ATOM 2492 O GLU 309 25.287 50.180 -9.826 1.00 14.89 ATOM 2493 N PRO 310 27.164 49.735 -10.842 1.00 14.73 ATOM 2493 CD PRO 310 28.275 50.012 -11.799 1.00 16.91 ATOM 2496 CB PRO 310 28.275 50.012 -11.799 1.00 16.91 ATOM 2497 CG PRO 310 28.275 50.012 -11.799 1.00 16.91 ATOM 2498 C PRO 310 27.152 48.348 -10.386 1.00 17.03 ATOM 2497 CG PRO 310 28.7152 48.348 -10.386 1.00 17.03 ATOM 2497 CG PRO 310 28.7152 48.348 -10.386 1.00 17.03 ATOM 2497 CG PRO 310 28.7152 48.348 -10.386 1.00 17.03 ATOM 2498 C PRO 310 28.7152 48.348 -10.386 1.00 15.04 ATOM 2497 CG PRO 310 28.7152 48.348 -10.386 1.00 17.03 ATOM 2497 CG PRO 310 28.7152 48.348 -10.386 1.00 15.04 ATOM 2497 CG PRO 310 28.7152 48.348 -10.386 1.00 15.04 ATOM 2497 CG PRO 310 28.7152 48.348 -10.386 1.00 15.04 ATOM 2497 CG PRO 310 28.7152 48.366 -8.874 1.00 13.88	
ATOM 2479 CZ ARG 308 17.733 52.219 20.00 14.58 ATOM 2480 NH1 ARG 308 18.288 51.740 -9.404 1.00 19.03 ATOM 2481 NH2 ARG 308 16.517 52.713 -10.426 1.00 19.03 ATOM 2482 C ARG 308 24.511 52.680 -12.443 1.00 18.59 ATOM 2483 O ARG 308 25.055 52.218 -13.440 1.00 25.55 ATOM 2484 N GLU 309 25.070 52.659 -11.241 1.00 18.16 ATOM 2484 N GLU 309 25.070 52.659 -10.946 1.00 19.38 ATOM 2485 CA GLU 309 26.350 52.054 -10.946 1.00 19.38 ATOM 2486 CB GLU 309 27.058 52.935 -9.907 1.00 21.98 ATOM 2487 CG GLU 309 27.442 54.299 -10.501 1.00 30.05 ATOM 2488 CD GLU 309 27.442 54.299 -10.501 1.00 30.05 ATOM 2489 OE1 GLU 309 28.319 54.244 -11.731 1.00 30.05 ATOM 2490 OE2 GLU 309 28.114 55.058 -12.663 1.00 37.666 ATOM 2491 C GLU 309 26.233 50.607 -10.484 1.00 15.87 ATOM 2491 C GLU 309 25.287 50.180 -9.826 1.00 14.89 ATOM 2493 N PRO 310 27.164 49.735 -10.842 1.00 16.91 ATOM 2494 CD PRO 310 28.275 48.348 -10.386 1.00 17.03 ATOM 2495 CA PRO 310 28.275 48.348 -10.386 1.00 17.03 ATOM 2496 CB PRO 310 28.419 47.733 -11.059 1.00 17.03 ATOM 2496 CB PRO 310 28.710 48.625 -12.220 1.00 19.08 ATOM 2497 CG PRO 310 28.700 48.625 -12.220 1.00 19.08 ATOM 2497 CG PRO 310 28.700 48.665 -8.874 1.00 13.88	
ATOM 2480 NH1 ARG 308 15.203 -10.426 1.00 19.03 ATOM 2481 NH2 ARG 308 16.517 52.713 -10.426 1.00 18.59 ATOM 2482 C ARG 308 24.511 52.680 -12.443 1.00 18.59 ATOM 2483 O ARG 308 25.055 52.218 -13.440 1.00 25.55 ATOM 2484 N GLU 309 25.070 52.659 -11.241 1.00 18.16 ATOM 2485 CA GLU 309 26.350 52.054 -10.946 1.00 19.38 ATOM 2486 CB GLU 309 27.058 52.935 -9.907 1.00 21.98 ATOM 2486 CB GLU 309 27.058 52.935 -9.907 1.00 25.52 ATOM 2487 CG GLU 309 27.442 54.299 -10.501 1.00 25.52 ATOM 2488 CD GLU 309 28.319 54.244 -11.731 1.00 30.05 ATOM 2489 OE1 GLU 309 29.244 53.401 -11.842 1.00 36.16 ATOM 2490 OE2 GLU 309 28.114 55.058 -12.663 1.00 37.66 ATOM 2491 C GLU 309 26.233 50.607 -10.484 1.00 15.87 ATOM 2491 C GLU 309 26.233 50.607 -10.484 1.00 15.87 ATOM 2492 O GLU 309 25.287 50.180 -9.826 1.00 14.89 ATOM 2493 N PRO 310 27.164 49.735 -10.842 1.00 14.73 ATOM 2494 CD PRO 310 28.275 50.012 -11.799 1.00 16.91 ATOM 2495 CA PRO 310 28.275 50.012 -11.799 1.00 16.91 ATOM 2496 CB PRO 310 28.419 47.733 -11.059 1.00 17.03 ATOM 2497 CG PRO 310 28.419 47.733 -11.059 1.00 17.03 ATOM 2498 C PRO 310 28.700 48.625 -12.220 1.00 19.09	
ATOM 2481 NH2 ARG 308 16.517 52.680 -12.443 1.00 18.59 ATOM 2482 C ARG 308 24.511 52.680 -12.443 1.00 25.55 ATOM 2483 O ARG 308 25.055 52.218 -13.440 1.00 25.55 ATOM 2484 N GLU 309 25.070 52.659 -11.241 1.00 18.16 ATOM 2485 CA GLU 309 27.058 52.935 -9.907 1.00 21.98 ATOM 2486 CB GLU 309 27.058 52.935 -9.907 1.00 25.52 ATOM 2487 CG GLU 309 27.442 54.299 -10.501 1.00 30.05 ATOM 2488 CD GLU 309 28.319 54.244 -11.731 1.00 30.05 ATOM 2488 CD GLU 309 29.244 53.401 -11.842 1.00 36.16 ATOM 2489 OE1 GLU 309 28.114 55.058 -12.663 1.00 37.66 ATOM 2490 OE2 GLU 309 28.114 55.058 -12.663 1.00 37.66 ATOM 2491 C GLU 309 26.233 50.607 -10.484 1.00 15.87 ATOM 2492 O GLU 309 25.287 50.180 -9.826 1.00 14.89 ATOM 2493 N PRO 310 27.164 49.735 -10.842 1.00 16.91 ATOM 2493 N PRO 310 27.164 49.735 -10.842 1.00 16.91 ATOM 2494 CD PRO 310 28.275 50.012 -11.799 1.00 16.91 ATOM 2495 CA PRO 310 28.419 47.733 -11.059 1.00 17.03 ATOM 2496 CB PRO 310 28.419 47.733 -11.059 1.00 17.03 ATOM 2497 CG PRO 310 28.419 47.733 -11.059 1.00 17.03 ATOM 2498 C PRO 310 28.700 48.625 -12.220 1.00 19.09	
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ATOM 2497 CG PRO 310 28.700 10.00 13.88 ATOM 2498 C PRO 310 27.219 48.266 -8.874 1.00 15.60	
2498 C PRO 310 27.219 to 268 -8 164 1.00 15.60	
ATOM 2499 0 PRO 310 27.441 47.318 -8.360 1.00 12.14	
ATOM 2500 N LEU 311 26 328 47 085 -6.922 1.00 11.23	
ATOM 2501 CA LEU 311 24.878 47.460 -6.615 1.00 13.50	
ATOM 2502 CB LEU 311 21 47 333 -5.180 1.00 13.50	
ATOM 2503 CG LEU 311 25 139 48.120 -4.233 1.00 20.1	
ATOM 2504 CD1 LEU 311 22.986 47.700 -5.047 1.00 17.3	
ATOM 2505 CD2 LEU 311 26.572 45.604 -6.622 1.00 11.7	
ATOM 2506 C 111 25 915 44.759 -7.247 1.00	
ATOM 2507 0 112 27.494 45.257 -5.728 1.00 11.3	
ATOM 2508 1 27.725 43.854 -5.407	
ATOM 2509 CA 312 29.040 43.653 -4.645 1.00 20.9	
ATOM 2510 05 SEP 312 28.821 43.933 -3.204	
ATOM 2311 C SER 312 26.576 43.311 2 200 11.1	8
ATOM 2512 O SER 312 26.000 44.059 1.00 9.0	6
ATOM 2514 N TYR 313 26.260 42.025 4152 1.00 8.5	6
ATOM 2515 CA TYR 313 25.095 41.471 1.00 9.0	
ATOM 2516 CB TYR 313 24.722 40.062 -4.375 1.00 7.5	
2517 CG TYR 313 23.255 1.00 8.1	
ATOM 2518 CD1 TYR 313 22.250 40.004 -5.038 1.00 8.1	
NTOM 2519 CEI TYR 313 20.951 40.05 -3.179 1.00 6.	
ATOM 2520 CD2 TYR 313 221 39.151 -2.889 1.00 0.	
ATOM 2521 CE2 TYR 313 20.558 39.481 -3.810 1.00 6.	
ATOM 2522 CZ TYR 313 19 227 39.413 -3.570 1.00 /.	88
ATOM 2523 On 113 25.247 41.465 -2.642 1.00	66
ATOM 2524 C TIN 313 24.295 41.721 -1.876	27
ATOM 2525 0 114 26.436 41.154 -2.137 1.00	
ATOM 2525 CD CLV 314 26.636 41.130	24
ATOM 2527 314 26.438 42.475 10.025	
ATOM 2528 GIV 314 25.837 42.532 1.044 1.00 12	52
ATOM 2525 N ASP 315 26.927 43.543 -0.636 1.00 13	51
ATOM 253 CD ASP 315 26.682 44.876 -0.115 1.00 11	.36
ATOM 2532 C ASP 315 25.178 45.169 0.871 1.00 12	. 03
ATOM 2523 O ASP 315 24.643 45.674 1.023 1.00 18	.60
ATOM 2534 CB ASP 315 27.367 45.515 -0.671 1.00 23	.51
ATOM 2535 CG ASP 315 28.845 46.015 0.214 1.00 34	.09
2536 OD1 ASP 315 29.300 45.875 -1.358 1.00 38	. 29
2537 OD2 ASP 315 23.110 100 100 100 100 100 100 100 100 100	. 83
ATOM 2538 N TYR 316 24.536 45.065 -1.383 1.00	.46
ATOM 2539 CA TYR 316 23.621 44.578 -2.740 1.00	. 26
ATOM 2540 CB 11k 21 120 44 397 -2.840 1.00	.60
ATOM 2541 CG 11R 320 272 45 477 -3.037 1.00	3.34
ATOM 2542 CD1 117 316 18 913 45.293 -3.143 1.00	7.74
ATOM 2543 CE1 TYR 316 20.585 43.119 -2.768 1.00	7.91 7.88
ATOM 2544 CD2 III 316 19.210 42.953 -2.847 1.00	7.84 7.84
ATOM 2545 CE2 TYR 316 18.381 44.028 -3.021 1.00	8.21
ATOM 2546 CZ 11K 316 17.021 43.799 -3.101 1.00	8.23
ATOM 2547 OR TYR 316 22.328 44.386 -0.283 1.00	8.68
ATOM 2548 C TYR 316 21.435 44.940 0.393 1.00	8.47
ATOM 2549 0 1511 317 22.637 43.104 -0.045	8.58
ATOM 2330 LEU 317 21.902 42.282	
ATOM 2551 CA 200	

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ATOM	2552	СВ	LEU						
ATOM	2553						0.743	1.00	8.79
ATOM	2554		_				1.629	1.00	8.20
ATOM	2555						1.272	1.00	9.81
ATOM	2556	C C	LEU				1.492	1.00	10.08
ATOM	2557	ō	LEU	31			2.352	1.00	8.90
ATOM	2558	N		31			3.087	1.00	9.53
ATOM	2559	CA	GLN	31		42.918	2.770	1.00	10.62
ATOM	2560		GLN	31		43.262	4.185	1.00	12.66
ATOM	2561	CB	GLN	31		43.337	4.464	1.00	
ATOM	2562	CG	GLN	31		43.620	5.905	1.00	14.04
ATOM	2563	CD	GLN	31		43.890	6.154	1.00	19.74
ATOM		OE1		31		44.211	5.249	1.00	23.96
ATOM	2564	NE2		31		43.856	7.426	1.00	35.18
ATOM	2565	C	GLN	318		44.561	4.553	1.00	29.80
ATOM	2566	0	GLN	318		44.673	5.560	1.00	12.86
ATOM	2567	N	ASN	319		45.524	3.641	1.00	15.11
ATOM	2568	CA	ASN	319		46.806	3.917	1.00	12.55
ATOM	2569	CB	ASN	319	23.012	47.860	3.043		14.03
ATOM	2570	CG	ASN	319	24.469	48.100	3.472	1.00	20.38
ATOM	2571	OD1	ASN	319	24.837	48.041	4.669	1.00	27.04
	2572	ND2	ASN	319	25.310	48.297	2.465	1.00	36.52
ATOM	2573	C	ASN	319	20.844	46.703	3.764	1.00	38.86
ATOM	2574	0	ASN	319	20.143	47.296	4.593	1.00	11.80
ATOM	2575	N	GLY	320	20.312	45.946	2.806	1.00	11.96
ATOM	2576	CA	GLY	320		45.829		1.00	9.58
ATOM	2577	С	GLY	320		45.194	2.624	1.00	9.89
ATOM	2578	0	GLY	320		45.598	3.797	1.00	9.39
ATOM	2579	N	LEU	321		44.151	4.167	1.00	10.40
ATOM	2580	CA	LEU	321		43.464	4.363	1.00	9.14
ATOM	2581	CB	LEU	321	18.857		5.485	1.00	9.96
ATOM	2582	CG	LEU	321	18.723	42.133	5.768	1.00	10.64
ATOM	2583	CD1	LEU	321	19.399	41.078	4.638	1.00	10.47
ATOM	2584	CD2	LEU	321	17.262	39.826	5.109	1.00	15.39
ATOM	2585	С	LEU	321		40.824	4.233	1.00	12.12
ATOM	2586	0	LEU	321	18.108	44.339	6.710	1.00	10.07
ATOM	2587	N	VAL	322	17.089	44.340	7.437	1.00	10.21
MOTA	2588	CA	VAL	322	19.176	45.095	6.956	1.00	10.17
ATOM	2589	CB	VAL		19.146	46.035	8.069	1.00	11.92
ATOM	2590	CG1	VAL	322	20.532	46.687	8.252	1.00	14.76
ATOM	2591	CG2	VAL	322	20.397	47.770	9.346	1.00	20.10
ATOM	2592	C	VAL	322	21.537	45.651	8.753	1.00	21.00
ATOM	2593	0		322	18.095	47.100	7.854	1.00	10.68
ATOM	2594	и.	VAL	322	17.346	47.521	8.741	1.00	12.21
ATOM	2595	CA	SER	323	18.014	47.617	6.634	1.00	11.81
ATOM	2596	CB	SER	323	17.069	48.683	6.345	1.00	11.28
ATOM	2597	OG	SER	323	17.295	49.233	4.922	1.00	14.31
ATOM	2598		SER	323	18.592	49.829	4.835	1.00	19.95
ATOM	2599	C	SER	323	15.625	48.220	6.522	1.00	11.18
ATOM	2600	0	SER	323	14.776	48.982	6.976	1.00	
ATOM	2601	N	LEU	324	15.345	46.979	6.128	1.00	12.09
ATOM	2602	CA	LEU	324	13.986	46.458	6.212	1.00	11.02
ATOM		CB	LEU	324	13.893	45.156	5.430	1.00	9.92
ATOM	2603	CG	LEU	324	12.522	44.506	5.348	1.00	9.96
ATOM	2604	CD1	LEU	324	11.448	45.393	4.776	1.00	9.98
ATOM	2605	CD2	LEU	324	12.658	43.214	4.571	1.00	11.33
ATOM	2606	C	LEU	324	13.576	46.326	7.679	1.00	11.39
ATOM	2607	0	LEU	324	12.422	46.540	8.070		10.28
	2608	N	ILE	325	14.532	45.886	8.497	1.00	10.32
ATOM	2609	CA	ILE	325	14.292	45.805	9.939	1.00	10.22
ATOM	2610	CB	ILE	325	15.451	45.120	10.669	1.00	11.04
ATOM	2611	CG2	ILE	325	15.398	45.298		1.00	10.87
ATOM	2612	CG1	ILE	325	15.454	43.605	12.164	1.00	13.93
ATOM	2613	CD1	ILE	325	16.785	42.944	10.363	1.00	12.46
ATOM	2614	C	ILE	325	14.040	47.192	10.725	1.00	15.56
ATOM	2615	0	ILE	325	13.122	47.192	10.522	1.00	10.74
ATOM	2616	N	ASN	326	14.819		11.341	1.00	11.60
ATOM	2617	CA	ASN	326	14.602	48.181	10.151	1.00	10.99
ATOM	2618	CB	ASN	326	15.732	49.531	10.659	1.00	12.82
ATOM	2619	CG	ASN	326	17.014	50.459	10.168	1.00	14.29
ATOM	2620	OD1	ASN	326		50.101	10.904	1.00	17.21
ATOM	2621	ND2	ASN	326	16.959	49.382	11.917	1.00	23.79
ATOM	2622	C	ASN	326	18.130	50.520	10.318	1.00	22.06
ATOM	2623		ASN	326	13.265	50.066	10.203	1.00	12.41
ATOM	2624		LYS	325	12.620	50.749	10.996	1.00	14.07
				341	12.840	49.790	8.973	1.00	11.71

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								0.469	1.00	12.41
				327	11.58	36 5	50.307	8.468	1.00	13.45
ATOM	2625	CA	LYS		11.54		50.205	6.918		18.26
ATOM	2626	CB	LYS		10.36	-	50.865	6.259	1.00	21.08
	2627	CG	LYS	327			50.144	5.014	1.00	21.51
MOTA	2628	CD	LYS	327	9.84	• •	50.768	4.423	1.00	
ATOM	2629	CE	LYS	327	8.60	• •	50.650	5.211	1.00	17.68
ATOM		NZ	LYS	327	7.3			9.067	1.00	11.15
ATOM	2630		LYS	327	10.3	3/	49.653	9.506	1.00	12.52
ATOM	2631	C	LYS	327	9.3	89	50.327	8.990	1.00	10.58
MOTA	2632	0		328	10.3	58	48.303		1.00	11.33
ATOM	2633	M	ASN	328	9.1		47.510	9.286	1.00	14.02
ATOM	2634	CA	ASN		8.7		46.614	8.084	1.00	14.11
	2635	CB	ASN	328	8.0		47.438	7.002		16.02
ATOM	2636	CG	ASN	328			48.681	7.112	1.00	
MOTA	2637	OD1	ASN	328	7.5		46.796	5.995	1.00	11.03
MOTA		ND2	ASN	328		525		10.551	1.00	11.26
MOTA	2638	C	ASN	328	9.7		46.671	10.873	1.00	13.57
ATOM	2639		ASN	328	8.3	226	45.994	11.270	1.00	12.34
MOTA	2640	0		329	10.	341	46.732		1.00	12.29
MOTA	2641	N	GLY	329	10.		46.076	12.554	1.00	11.30
ATOM	2642	CA	GLY		11.		44.739	12.523	1.00	11.94
ATOM	2643	С	GLY	329		221	44.056	11.517		11.96
	2644	0	GLY	329			44.359	13.668	1.00	
MOTA	2645	N	GLN	330		716	43.036	13.787	1.00	10.55
MOTA		CA	GLN	330		364		15.072	1.00	11.32
ATOM	2646	CB	GLN	330		.193	42.950	15.352	1.00	11.79
ATOM	2647		GLN	330	13	.686	41.560		1.00	10.04
MOTA	2648	CG		330		.755	41.131	14.371	1.00	13.20
MOTA	2649	CD	GLN	330	_	.804	41.744	14.168	1.00	11.43
ATOM	2650	OE1	GLN			.469	40.024	13.733		10.94
	2651	NE2	GLN	330			41.961	13.747	1.00	12.29
MOTA	2652	С	GLN	330		.291	41.952	14.592	1.00	
ATOM		0	GLN	330		.401		12.784	1.00	9.93
MOTA	2653	N	THR	331	11	377	41.063	12.692	1.00	10.56
MOTA	2654		THR	337	10	.438	39.956	11.277	1.00	13.12
MOTA	2655	CA		333	1 10	.367	39.375	11.277	1.00	14.79
ATOM	2656	CB	THR	33		1.627	38.829	10.872	1.00	18.32
ATOM	2657	OG1				9.945	40.455	10.274	1.00	9.68
	2658	CG2		33	_	0.801	38.843	13.669	1.00	10.45
ATOM	2659	С	THR	33	-		37.874	13.694	1.00	9.25
MOTA	2660	0	THR	33	_	9.996	38.971	14.419	1.00	
MOTA		OT	THR	33		1.803		-0.715	1.00	6.49
MOTA	2661	OW	WAT	33	3	9.679	28.766	10.936	1.00	7.24
ATOM	2662			3.3	4 1	9.171	27.783	-4.195	1.00	8.08
MOTA	2663	WO		3 3		9.260	43.735	2.029	1.00	6.26
ATOM	2664	OM		33		2.532	31.208		1.00	7.97
MOTA	2665	OM				8.595	34.041	1.151	1.00	8.47
MOTA	2666	OW				4.607	26.075	6.861		8.55
ATOM	2667	OW			-	-2.784	36.461	-0.561	1.00	7.69
	2668	OV	TAW U				23.031	7.059	1.00	8.58
MOTA	2669	OV	raw ,	3	-	22.156	39.110	1.828	1.00	
MOTA				3		14.777		1.589	1.00	9.25
MOTA	2670					12.607	41.059	12.742	1.00	9.09
MOTA	2671					-1.547	35.753	12.366	1.00	8.72
MOTA	2672			_	44	15.859	16.926	2.078	1.00	8.11
MOTA	2673	_	· ·		345	17.270	37.486		1.00	10.08
ATOM	2674	-		-	346	3.657	33.965	-24.602	1.00	9.87
ATOM	2679	-	AW WA	•	347	25.532	21.232	-3.227	1.00	9.24
ATOM	2676	6 0	AW W	-		-2.697		10.127		
ATOM	267	_	AW WO		348	-1.983	- 0 140	8.911	1.00	
	267	_	AW WO		349			10.377	1.00	20
MOTA	267		W.F	T	350	2.708			1.00	1
MOTA			W WC	T	351	1.466		_	1.00	10.21
MOTA	268				352	1.694	36.486		1.00	11.32
MOTA	268	-		AT	353	14.78	7 40.054		1.00	11.49
MOTA	268				354	7.94			1.00	
MOTA	268		•	AT	355	10.89	8 19.364	-0.933	- 0	
MOTA	268	34	O.,	AT		11.24	6 44.07	8.852	_	•
ATOM	268		.	AT	356	19.83		23.876		
			OM M	AT	357				1.0	•
MOTA				TA	358	27.71		9 -5.869	1.0	
MOTA				TAI	359	25.37		·	1.0	
MOTA				TAI	360	7.71				0 10.19
MOTA		89	· .	TAN	361	12.90				10.84
ATOM		90		TAN	362	15.46	65 41.81	· -	-	12.37
MOTA		91	· · · ·		363	12.3	47 17.85		•	
MOTA		592	U	TAN	364	16.3	02 36.64	-24.73	-	
MOTA		593	Q	TAW			65 30.65	51 24.02	•	
ATO		594	Q11	TAW	365			18 -15.//	-	
	·	695	OW .	TAW	366			61 10.95		
ATO		696	OM .	TAW	367			2 70	14.	00 11.14
ATO		697	OW	WAT	368	6.2		-		
OTA	m 2	, ,								

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ATOM		_	raw v	3	69 16.6	75 14 02			
ATOM	269			3	70 7.90		~	1.00	11.88
ATOM	270		/ WAT	' 3	71 18.36		_	1.00	10.25
ATOM	270		YAT		72 21.89			1.00	
ATOM	270	2 OW	WAT		73 7.41	_	051	1.00	
ATOM	270	3 OW	WAT		74 9.30		-5.250	1.00	
ATOM	270	4 OW		_		_		1.00	
ATOM	270	5 OW		-				1.00	12.75
ATOM	270	5 OW		3 7				1.00	
ATOM	270							1.00	13.18
ATOM	2708		WAT	37			5.991	1.00	13.37
ATOM	2709		WAT	37				1.00	13.42
ATOM	2710		WAT	38			11.626	1.00	13.43
ATOM	2711			38			9.550	1.00	13.60
ATOM	2712		WAT	38		35.948	12.107	1.00	13.85
ATOM	2713		WAT	38			22.628		11.77
ATOM	2714		WAT	38		19.425	20.724	1.00	15.24
ATOM	2715		WAT	38		39.497	8.314	1.00	14.52
ATOM	2716	OW	WAT	38		45.847	-10.066	1.00	14.01
ATOM	2717	OW	WAT	38	7 -0.150	40.151	13.142	1.00	13.62
ATOM		OW	WAT	388	3 17.528	29.411	-23.847	1.00	15.04
ATOM	2718	OW	WAT	389	11.478		-25.585	1.00	12.67
ATOM	2719	OW	WAT	390	13.559			1.00	14.89
ATOM	2720	OW	WAT	391	8.290		10.705	1.00	15.14
ATOM	2721	OW	WAT	392		43.137	-0.320	1.00	13.16
	2722	OW	WAT	393		20.811	-23.378	1.00	13.36
ATOM	2723	OW	WAT	394		48.525	-4.126	1.00	14.45
ATOM	2724	OW	WAT	395			1.433	1.00	13.51
ATOM	2725	OW	WAT	396		28.028	-11.200	1.00	16.03
ATOM	2726	OW	WAT	397		33.285	2.180	1.00	13.36
ATOM	2727	OW	WAT	398	7.685	37.842	-7.595	1.00	14.72
ATOM	2728	OW	WAT	399	-2.609	39.106	-0.476	1.00	13.04
ATOM	2729	OW	WAT	400		52.730	2.926	1.00	15.18
ATOM	2730	OW	WAT	401	31.148	33.765	-2.024	1.00	15.90
ATOM	2731	OW	WAT	402	28.412	25.681	-6.948	1.00	14.37
MOTA	2732	OW	WAT	403	-7.837	33.960	-2.251	1.00	16.42
ATOM	2733	OW	WAT	404	27.733	30.817	11.858	1.00	
ATOM	2734	OW	WAT		20.345	47.455	-0.111	1.00	16.15
ATOM	2735	OW	WAT	405	7.740	46.885	-13.836	1.00	15.84
ATOM	2736	OW	WAT	406	-6.948	43.028	7.219	1.00	15.47
ATOM	2737	OW	WAT	407	-1.255	31.160	-1.492	1.00	13.61
ATOM	2738	OW		408	-7.351	47.298	1.758	1.00	15.03
ATOM	2739	OW	TAW	409	0.600	50.511	3.412		16.16
ATOM	2740	OW	WAT	410	19.491	38.870	14.832	1.00	16.57
ATOM	2741		WAT	411	19.032	29.394	25.238	1.00	13.70
ATOM	2742	OM	WAT	412	1.566	19.249	-3.495	1.00	13.82
ATOM	2742	OW	WAT	413	1.396	29.458	-19.005	1.00	12.61
ATOM	2743	OW	WAT	414	12.993	13.760	6.156	1.00	17.83
ATOM		OW	WAT	415	-3.489	25.740	2.588	1.00	16.00
ATOM	2745	OW	WAT	416	20.400	16.258	4.749	1.00	14.57
ATOM	2746	OW	WAT	417	8.420	43.590	11.063	1.00	15.12
ATOM	2747	OW	TAW	418	23.155	21.243	-11.863	1.00	15.17
ATOM	2748	OM	WAT	419	13.407	49.512	-4.704	1.00	15.01
ATOM	2749	OW	WAT	420	2.293	43.872	-6.246	1.00	18.08
	2750	OW	WAT	421	16.464	23.984	-19.188	1.00	15.75
ATOM	2751	OW	WAT	422	18.051	10 401	-12.729	1.00	16.55
ATOM	2752	OW	WAT	423	2.749	18.401	13.304	1.00	16.18
ATOM	2753	OW	WAT	424	3.167	32.610	17.294	1.00	16.03
ATOM	2754		WAT	425		43.048	-21.870	1.00	16.60
ATOM	2755		WAT	426	1.729	36.092	20.156	1.00	16.00
ATOM	2756		WAT	427	24.912	30.437	18.039	1.00	18.10
ATOM	2757		WAT		1.661	37.179	-17.778	1.00	
ATOM	2758		TAW	428	8.377	48.751	-17.456	1.00	16.68
ATOM	2759		WAT	429	4.193	48.686	-6.577	1.00	17.96
ATOM	2760			_	32.183	20.100	4.650	1.00	16.18
ATOM	2761				10.701	20.889	-9.309		17.47
ATOM	2762	-		432	1.230	36.624	-21.785	1.00	17.06
ATOM	2763				23.224	53.219	-9.124	1.00	16.21
ATOM	2764			434	7.454	14.204	-2.641	1.00	16.77
ATOM	2765				3.493	18.204	-1.008	1.00	19.16
ATOM	2766				28.871	35.527	-9.186	1.00	16.26
ATOM				437 2	8.827	47.359	-4.440	1.00	16.44
ATOM	2767			138]	.6.179	24.748	-15.541	1.00	20.15
ATOM	2768				4.130	23.189	10.125	1.00	18.41
ATOM	2769			40	9.413	18.353	13 215	1.00	15.71
-11 01-1	2770	OW W	AT 4	41	8.848	18.233	13.315	1.00	22.18
					_		10.527	1.00	19.65

WO 98/16648										
					•			. 2 217	1.00	16.18
			WAT	442	26.464	32.		18.217 4.061	1.00	17.91
ATOM	2771	OM.	TAW		-7.877	38.		10.130	1.00	14.21
ATOM	2772	OM	WAT		12.963	34.		16.871	1.00	17.53
ATOM	2773	OM	TAW	445	5.117	7 27.	600	2.096	1.00	20.90
ATOM	2774	OM	TAW	446	-9.839	37.	847	3.793	1.00	20.56
ATOM	2775	OM	WAT	447	-1.74	5 32.	409	9.538	1.00	19.37
MOTA	2776	OM	TAW	448	8.41	_	.915	0.805	1.00	15.63
ATOM	2777	OM	TAW	449	13.44	_	.906	20.352	1.00	16.16
MOTA	2778	OM	TAW	450	4.45	•	.452	-0.627	1.00	17.14
ATOM	2779	OM	WAT	451	8.79		.265	21.516	1.00	17.26
MOTA	2780	OW	TAW	452	-0.35	6 37	.156	-22.757	1.00	21.00
MOTA	2781	OM	WAT	453	11.47	17 23	.152	24.676	1.00	18.12
ATOM	2782	OW	TAW	454	21.49	90 29	.901	10.367	1.00	20.23
ATOM	2783	OW	TAW	455	-9.43	38 38	.109	-6.497	1.00	16.76
MOTA	2784	OM	TAW	456	0.8		.803	-14.695	1.00	19.53
MOTA	2785	OM	TAW	457	19.9		.749	19.711	1.00	20.63
ATOM	2786	OW	TAW	458	15.6	65 20	.950	7.507	1.00	18.83
MOTA	2787	OM	TAW	459	22.2	53 43	2.588	-0.991	1.00	17.62
MOTA	2788	OM	TAW	460	1.0		5.140	-1.171	1.00	18.28
ATOM	2789	OW	TAW	461	15.0		7.428	19.798	1.00	19.90
ATOM	2790	OW	T'AW	462	9.2		6.847	12.465	1.00	20.21
MOTA	2791	OW	WAT	463	23.4	158 3	1.087	9.231	1.00	20.50
MOTA	2792	WO	WAT	464	19.9		2.399	-1.994	1.00	18.86
MOTA	2793	OW	TAW	465	-1.	338 2	2.340	-7.395	1.00	20.44
MOTA	2794	OW	WAT	466	3.	252 2	20.298	-27.095	1.00	19.91
MOTA	2795	WO	TAW	467	13.	042	53.167	15.133	1.00	20.65
MOTA	2796	OW	TAW	468	-10.	9	37.955	-8.488	1.00	20.52
ATOM	2797	OW		469			21.680	9.484	1.00	17.30
MOTA	2798	WO		470	10.	200	15.611	-27.728	1.00	15.98
MOTA	2799	OW		471	18.	30-	39.511	-0.891	1.00	18.92
MOTA	2800	OW		472		.497	24.989	11.353	1.00	20.62
MOTA	2801	OW		473	3 34	.106	27.545	-1.003	1.00	21.04
ATOM	2802	OV OV		47		.263	34.235	8.033	1.00	22.42
MOTA	2803	OV OV	·	47	5 30	.740	34.281	-24.851	1.00	19.76
ATOM	2804	O		47		.888	47.600	-22.920	1.00	19.37
MOTA	2805	01				.023	45.815	-23.488	1.00	23.73
MOTA	2806					.376	27.996	13.239	1.00	19.22
ATOM	2807					3.268	40.811	-11.498	1.00	18.91
MOTA	2808	-			30 -4	.271	44.290	1.254	1.00	19.73
MOTA	2809				31 -10	0.443	35.240	20.144	1.00	19.18
ATOM	2810					2.681	33.500	12.144	1.00	20.32
ATOM	2811	•	,		83 1	9.770	15.947	7.499	1.00	21.46
MOTA	2812					4.713	13.467	-0.398	1.00	
MOTA	281	_			0 -	8.355	31.805	2.640	1.00	18.04
MOTA	281	-	AW WC AW WO		86 1	5.331	47.230	8.919	1.00	
MOTA	281	-	OW WA	_	87 2	5.206	36.975	14.409	1.00	0 18.16
MOTA	281	. •	. 1.17		88	2.787	39.754	-9.024	1.00	
MOTA	281	•	OM ME		189	2.364	46.924	-26.268	1.0	0 19.59
ATOM	281		OW W		190	18.912	42.320	-7.989	1.0	
MOTA	281		•••		491	9.332	14.150		1.0	
MOTA	282		011		492	3.716	51.522		1.0	
MOTA	28		•••		493	30.485	19.369	7 529	1.0	00 21.63
MOTA	28		O++		494	-8.748	45.801 16.205		1.0	1
MOTA	28		O.,	AT	495	11.868	35.997		1.0	05
MOTA		24	O.,	AT	496	13.346	40.899		1.0	
MOTA		25	O.,	TAI	497	0.972	53.53) 1.	
MOTA		126	U11	TA	498	4.183	39.01		5 1.	
MOTA		327		TAI	499	30.346	24.51) 1.	00 25.21
MOTA		328	0	TAN	500	16.129	41.63		91.	00 28.12
MOTA	•	829	O.,	TAW	501	10.923	24.86		4 1.	00 22.89 00 19.20
MOTA	1	830	O	TAW	502	18.809	14.11		1 1.	70
ATON	•	831	0,,	TAW	503	16.648	39.70		9 1.	01
OTA	• •	832	0	TAW	504	19.213	56.54	,	.8 1	
ATO		833	OM	TAW	505	24.711	29.5	-23.67	77 1	.00 22.77
ATO:	1.1	834	OM OM	TAW	506			20.01	51 ¹	.00 24.26
OTA	4.4	2835	OM	TAW	507	21.631	41.0° 32.9	· -	55 1	.00 25.98
ATO	/4.1	2836	OM	TAW	. 508	-3.925			67 1	.00 23.91
ATC	/1.1	2837	OM OM	WAT	509	-3.683			89 1	00 24.78
ATO	J1-1	2838	OW	WAT	510	22.548	22.9		64 1	1.00 21.05
ATO	J1-1	2839	OW	WAT	511	3.233	21.6		28	1.00 24.54
ATC	МО	2840	OM	WAT	512				78	1.00 25.43
AT	OM	2841	OM .	WAT	513	24.602	•	, 20		1.00 22.61
TA		2842	OW	WAT	514	16.68	b 43.8			•
AT	MO	2843	J							

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ATOM	1 21	844	OW N	VAT						
ATOM	28	345			515	10.96	-0.5,	6 -6.71		
ATOM	28	346		AT	516	0.840	16.58	2 -3.289		-0.05
ATOM		147	_	AT	517	-3.923	22.46	4 -1.744		~~ 2
ATOM		148	· · ·	AT	518	-0.997	25.90		\	00 29.01
ATOM		49		AT	519	3.066	45.06			00 27.67
ATOM				AT	520	20.631	16.30			30 21.23
ATOM		50		ΑT	521	3.683	28.042		1.0	0 29.84
ATOM	28		OW W.	AT	522	-7.926			1.0	
	28		OW W	AΤ	523			2.011	1.0	
ATOM	28	53			524	1.150	23.857	7 -9 846	1.0	
ATOM	289	54		_		13.889	16.199	-5.074	1.0	/1
ATOM	289	5 5	OW W.		525	-1.704	53.692	-2.952		
ATOM	289		OW WZ	_	526	30.576	35.496	-4.718	1.0	-2.07
ATOM	285			_	527	7.959	27.774	-32.333	1.00	
ATOM	285			_ `	528	0.310	39.649	-17.650	1.00	05
ATOM	285				529	-0.573	40.681		1.00	
ATOM	286			-	530	-5.413	37.314		1.00	24.02
ATOM	286	_	AW WC		31	20.453	25.296	-11.579	1.00	26.13
ATOM			AW WG	_	32	2.287	15.472	-22.221	1.00	26.01
ATOM	286		W WA	r 5	33	30.000		-5.046	1.00	27.90
ATOM	286	_	W WA:	r 5	_	13.014	42.526	-1.756	1.00	25.99
	2864		W WAT			19.089	48.338	13.867	1.00	-0.55
ATOM	2869		W WAT	_	'		59.470	-16.490	1.00	-7.73
ATOM	2866	5 0			`	23.246	37.608	-22.518	1.00	25.60
ATOM	2867	7 01				18.012	23.775	-22.832		30.37
ATOM	2868			-		32.942	31.103	-1.587	1.00	35.14
ATOM	2869			-		24.244	39.395	8.376	1.00	27.55
ATOM	2870			_	10 1	6.151	39.516	11.126	1.00	25.84
ATOM	2871		_	54	11 -	9.496	38.640		1.00	27.39
ATOM	2872	-		54	2 1	1.570	53.681	6.232	1.00	23.00
ATOM		•		54	3	5.652	39.623	-24.197	1.00	25.04
ATOM	2873	ON		54		5.243	53.023	9.901	1.00	24.86
ATOM	2874	OW	WAT	54	5 2	1.732	51.336	-7.590	1.00	31.58
	2875	OW	WAT	54	6 24	5.109	45.731	-22.796	1.00	
ATOM	2876	OW	WAT	54	7 6	3.109	29.562	15.747	1.00	25.40
ATOM	2877	OW		54	0 10	5.300	48.774	10.712	1.00	26.48
ATOM	2878	OW				5.333	19.082	-6.041		22.97
ATOM	2879	OW		54:		1.477	39.693	-0.433	1.00	31.87
ATOM	2880	OW		550		.307	28.802	-2.454	1.00	24.27
ATOM	2881	OW	WAT	553	16	.750	23.348	20.119	1.00	28.07
ATOM	2882		WAT	552		.254	45.692	25.119	1.00	30.93
ATOM	2883	OW	WAT	553	7	.615	43.287	23.110	1.00	30.02
ATOM		OW	WAT	554		.139	41.273	12.031	1.00	31.35
ATOM	2884	OW	WAT	555		.531		15.275	1.00	24.54
ATOM	2885	OW	WAT	556		.562	43.159	1.000	1.00	28.18
	2886	OW	WAT	557		.748	35.560	22.961	1.00	25.96
ATOM	2887	OW	WAT	558		. 358	24.192	-10.428	1.00	
ATOM	2888	OW	WAT	559			13.845	7.421	1.00	29.93
ATOM	2889	OW	WAT	560		144	26.300	-1.473	1.00	24.97
ATOM	2890	OW	WAT			711	42.085	-22.328		23.51
MOTA	2891	OW	WAT	561		258	55.289	-14.564	1.00	27.47
ATOM	2892	OW		562		683	49.398	-2.033	1.00	25.35
ATOM	2893	OW	WAT	563	21.	974	39.944	7.537	1.00	27.95
ATOM	2894	OW	WAT	564	14.	094	24.261	-29.685	1.00	24.21
ATOM	2895		WAT	565	8.	391	16.742	16 503	1.00	30.81
ATOM	2896	OW	WAT	566	34.9	902	40.206	16.583	1.00	33.63
ATOM	2897	OW	TAW	567	7.2	246	39.309	3.922	1.00	34.09
ATOM		OW	WAT	568	1.5	772	52.043	7.727	1.00	25.05
ATOM	2898	OW	WAT	569	-10.3		35.406	-7.936	1.00	33.11
ATOM	2899	OW	WAT	570	19.0		33.406	-1.420	1.00	28.71
	2900	OW	WAT	571	25.1		21.727	-6.972	1.00	31.14
ATOM	2901	OW	WAT	572	-0.4		25.032	13.807	1.00	
ATOM	2902	OW	WAT	573		_	22.506	0.681	1.00	29.45
ATOM	2903	OW	WAT	574	7.5		13.615	9.613	1.00	29.75
ATOM	2904	OW	WAT		0.7	41	L 5 .993	-6.797		25.51
ATOM	2905	OM.		575	4.5	24 2	26.932	19.683	1.00	28.22
ATOM	2906		WAT	576	24.2	17 3	11.560	29.964	1.00	30.25
ATOM	2907	OW	WAT	577	-9.8	86 3	8.987	-0.391	1.00	30.98
ATOM	2908	OW	WAT	578	18.20	64 4	8.710	-0.391	1.00	30.58
ATOM		OW	WAT	579	7.09		8.558	-5.256	1.00	26.25
ATOM	2909	OW	WAT	580 -	11.40			-19.857	1.00	30.55
	2910	OW	WAT	581	0.23		8.772	12.578	1.00	23.49
ATOM	2911	OW	WAT		34.49	_	3.067	3.666	1.00	
ATOM	2912	OW	WAT	583			0.211	11.953	1.00	32.85
ATOM	2913	OW	WAT		-8.88		0.085	8.563	1.00	30.38
ATOM	2914	OW	WAT		19.64	-	6.274	-1.256		20.61
ATOM	2915	OW .	WAT	585	0.78		3.240	6.163	1.00	32.05
ATOM	2916	OW		586	6.77	2 16	5.061	19.133	1.00	28.48
		J.,	WAT	587	17.57	2 48	3.350	-0.455	1.00	28.67
								V.335	1.00	31.70

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MOTA	2917	OW	WAT	588	19.914	42.743	12.082	1.00	29.47
ATOM	2918	OW	WAT	589	28.293	43.369	3.095	1.00	41.10
ATOM	2919	OW	WAT	590	4.140	16.905	-6.015	1.00	33.04
ATOM	2920	OW	TAW	591	-7.536	49.473	0.700	1.00	26.21
ATOM	2921	OW	TAW	592	16.545	11.527	7.703	1.00	35.77
ATOM	2922	OW	WAT	593	21.751	26.587	-18.455	1.00	36.98
ATOM	2923	WO	WAT	594	28.027	36.486	9.408	1.00	30.24
ATOM	2924	OW	WAT	595	-3.668	27.781	16.465	1.00	32.59
ATOM	2925	OW	TAW	596	6.641	50.716	9.132	1.00	30.57
ATOM	2926	OW	WAT	597	14.904	54.419	-12.497	1.00	35.34
ATOM ATOM	2927	OW	TAW	598	13.687	41.518	18.737	1.00	28.20
ATOM	2928	OW	TAW	599	15.809	10.449	13.628	1.00	27.51
ATOM	2929	OW	WAT	600	0.266	35.585	-19.094	1.00	32.22
ATOM	2930	OW	WAT	601	1.157	32.250	-2.186	1.00	31.93
ATOM	2931 2932	OW	TAW	602	20.830	54.594	-22.978	1.00	38.78
ATOM	2933	OM	WAT	603	-6.482	24.335	0.209	1.00	27.40
ATOM	2934	OW	WAT	604	-0.221	24.757	-19.652	1.00	34.87
ATOM	2935	OW	WAT	605	4.475	41.359	13.507	1.00	38.95
ATOM	2936	OW	WAT WAT	606 607	18.365	17.118	-5.002	1.00	35.63
ATOM	2937	OW	WAT	608	10.129	37.103	7.607	1.00	37.59
ATOM	2938	OW	WAT	609	32.483	26.313	-6.257	1.00	34.83
ATOM	2939	OW	WAT	610	1.173	18.896	13.815	1.00	38.79
ATOM	2940	OW	TAW	611	21.714 16.630	21.650	-7.187	1.00	30.79
ATOM	2941	OW	WAT	612	3.332	13.196	3.673	1.00	38.22
ATOM	2942	OW	WAT	613	11.410	18.798	15.551	1.00	30.36
ATOM	2943	OW	WAT	614	1.890	46.061 53.075	15.908	1.00	30.96
ATOM	2944	OW	WAT	615	14.858	54.460	0.396	1.00	35.43
ATOM	2945	OW	WAT	616	27.164	22.302	-19.563	1.00	36.48
ATOM	2946	OW	TAW	617	25.844	30.643	9.178	1.00	28.96
ATOM	2947	OW	WAT	618	-11.773	30.992	13.3 7 3 19.536	1.00	37.70
ATOM	. 2948	OW	WAT	619	20.068	54.715	-26.556	1.00	35.27
ATOM	2949	OW	TAW	620	22.511	25.529	18.055	1.00	30.61
ATOM	2950	OW	WAT	621	4.762	24.578	19.147	1.00	39.02
MOTA	2951	OW	WAT	622	-5.809	31.212	-7.251	1.00	29.70 38.52
ATOM	2952	OM	WAT	623	2.302	46.734	-19.134	1.00	31.35
ATOM	2953	OW	WAT	624	-3.267	26.845	-9.657	1.00	26.55
MOTA	2954	OW	WAT	625	20.942	19.909	15.987	1.00	30.93
ATOM	2955	OW	WAT	626	14.335	19.417	27.897	1.00	41.36
ATOM	2956	OW	WAT	627	-8.960	44.991	2.623	1.00	32.33
ATOM	2957	OM	WAT	628	-2.896	18.495	3.945	1.00	33.15
ATOM	2958	OW	TAW	629	19.081	15.066	19.313	1.00	41.85
ATOM	2959	OW	WAT	630	26.583	40.965	-16.598	1.00	53.36
ATOM	2960	OW	WAT	631	9.201	30.845	-29.283	1.00	26.67
ATOM	2961	OW	WAT	632	29.771	29.232	13.030	1.00	37.22
ATOM ATOM	2962	OW	TAW	633	-9.063	44.258	5.485 -	1.00	30.64
ATOM	2963	OW	WAT	634	36.469	24.114	2.218	1.00	34.07
ATOM	2964 2965	OW	WAT	635	1.658	28.923	20.644	1.00	39.44
ATOM		OM	WAT	636	-8.637	37.196	-3.769	1.00	39.41
ATOM	2966 2967	ow ow	WAT	637	9.491	43.672	18.552	1.00	34.67
ATOM	2968	OW	WAT WAT	638	38.446	24.948	5.405	1.00	37.88
ATOM	2969	OW	WAT	639 640	16.362	21.306	-12.437	1.00	35.82
ATOM	2970	OM	WAT	641	11.407	51.004	-0.072	1.00	31.55
ATOM	2971	OW	WAT	642	38.229	24.335	8.085	1.00	39.89
ATOM	2972	OW	WAT	643	21.655 16.387	26.806	22.131	1.00	32.81
ATOM	2973	OW	WAT		-12.122	22.635	23.545	1.00	35.28
ATOM	2974	OW	WAT	645	-1.768	42.861 30.006	-8.757	1.00	43.21
ATOM	2975	OW	WAT	646	31.231	36.441	19.108	1.00	39.03
ATOM	2976	OW	WAT	647	-9.784	38.920	-7.964	1.00	40.74
ATOM	2977	OW	WAT	648	-5.666	31.659	18.620	1.00	37.25
ATOM	2978	OW	WAT	649	-2.584	54.436	21.328	1.00	32.24
ATOM	2979	OW	WAT	650	9.314	15.276	0.499 13.185	1.00	42.36
ATOM	2980	OW	WAT	651	20.108	12.329	9.346	1.00	41.13
ATOM	2981	OW	WAT	652	28.719	20.042	8.674	1.00	30.57
ATOM	2982	OW	WAT	653	27.567	35.432	11.915	1.00	30.27
ATOM	2983	OW	WAT	654	20.822	18.155	14.214	1.00 1.00	34.47
ATOM	2984	OW	WAT	655	-1.395	25.107	7.194	1.00	29.75
END						: /		1.00	42.08

 $\bar{\bar{C}}\text{O}_2$ C-3 exomethylene cephams with

hydrophobic side chains, e.g. $R = PhCH_2$, $R = PhOCH_2$,

 $R = HO_2C(CH_2)_4$

RCOHN

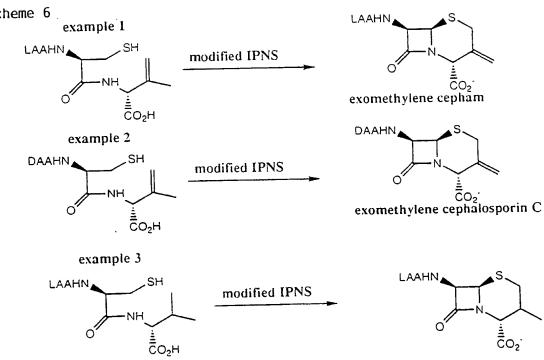
Scheme 2

7-aminocephalosporins

Scheme 5

where, R = alkyl or aryl or a combination of both, e.g. PHCH2, PhOCH2. The alkyl chain or aryl portion of R may also be substituted with acidic or basic groups, e.g. $R = HO_2C(CH_2)_4$, $R = H2N(CH_2)_4$. R may also be heterocyclic.

Scheme 6



Scheme 6 (cont.)

example 3 (cont.) The modified IPNS may be used in conjunction with another modified (or unmodified) enzyme activity, such as:

where R = LAA, DAA or other.

Scheme 7

example 1

example 2

H₃⁺N SH modified IPNS
$$\stackrel{\stackrel{}{=}}{=}$$
 $\stackrel{\stackrel{}{=}}{=}$ $\stackrel{\stackrel{}{=}}$

Scheme 8

example 1

example 2

example 1

modified or unmodified DAOCS, DACS or DAOC/DACS

where, R = aryl, alkyl or a combination of both e.g. $PhCH_2$, $PhOCH_2$. If R is alkyl it may be substituted, e.g. $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

example 2

where, R = aryl, alkyl or a combination of both e.g. $PhCH_2$, $PhOCH_2$. If R is alkyl it may be substituted, e.g. $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$. $R = D-\delta-(\alpha-aminoadipoyl)$.

examples

Scheme 11

example 1

where, $R = D-\delta-(\alpha-aminoadipoyl)$, $L-\delta-(\alpha-aminoadipoyl)$ $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

example 2

where, $R = D-\delta-(\alpha-aminoadipoyl)$, $D-\delta-(\alpha-aminoadipoyl)$ $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$, X = Cl, Br, I, OMe, SMe, or other substituent.

example 1

example 2

where R = CI, Br, I, OMe or other substituent.

Scheme 14

examples

where, R = aryl, alkyl or a combination of aryl and alkyl e.g. $PhCH_2$, $PhOCH_2$.

Scheme 12

example

other cephalosporins

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Scheme 15

examples

Scheme 16 example 1

where, $R = D-\delta-(\alpha-aminoadipoyl)$, $L-\delta-(\alpha-aminoadipoyl)$ $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$.

example 2

where, $R = D-\delta-(\alpha-aminoadipoyl)$, $D-\delta-(\alpha-aminoadipoyl)$ $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$, X = Cl, Br, I, OMe, SMe, or other substituent.

example 2

where R = Cl, Br, I, OMe or other substituent.

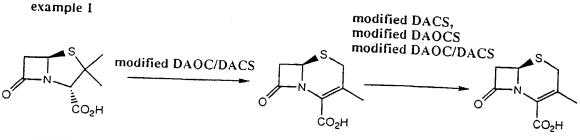
Scheme 19

examples

where, R = aryl, alkyl or a combination of aryl and alkyl e.g. $PhCH_2$, $PhOCH_2$.

Scheme 17

example



example 2

where R = Cl, Br, I, OMe or other substituent.

Scheme 23

examples

where, R = aryl, alkyl or a combination of aryl and alkyl e.g. $PhCH_2$, $PhOCH_2$.

Scheme 21

example

examples

Scheme 20

example 1

where, $R=D\text{-}\delta\text{-}(\alpha\text{-aminoadipoyl}),$ $L\text{-}\delta\text{-}(\alpha\text{-aminoadipoyl})$ $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4.$

example 2

where, $R=D-\delta$ -(α -aminoadipoyl), $D-\delta$ -(α -aminoadipoyl) $HO_2C(CH_2)_4$ or $H_2N(CH_2)_4$, X=Cl, Br, I, OMe, SMe, or other substituent.

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CLAIMS

- Isopenicillin N synthase (IPNS) in the form of: a complex with Mn having a structure designated by the X-ray co-ordinates in Table 2; or a complex with Fe and its substrate, said complex having a structure designated by the X-ray co-ordinates in Table 3.
- Isopenicillin N synthase (IPNS) in the form of: a complex with
 Fe and an analogue of its substrate, either in the absence or in the presence of nitrous oxide or dioxygen, said complex having a structure designated by X-ray co-ordinates analogous to that set out in Table 3.
 - 3. Use of the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for the modification of a second enzyme selected from IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway.
- 4. Use as claimed in claim 3, wherein the second enzyme is modified to accept unnatural substrates for the preparation of antibacterial materials or intermediate for the production of pharmaceutical products.
 - 5. Use as claimed in claim 3, wherein the second enzyme is modified to produce unnatural products or improve the production of natural products.
- 6. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:

R287; R87; R88; Y189; S183; Y91; F285; Q330; T331; V185; L106; C104; V217; L324; L317; I325; L321; S210.

10

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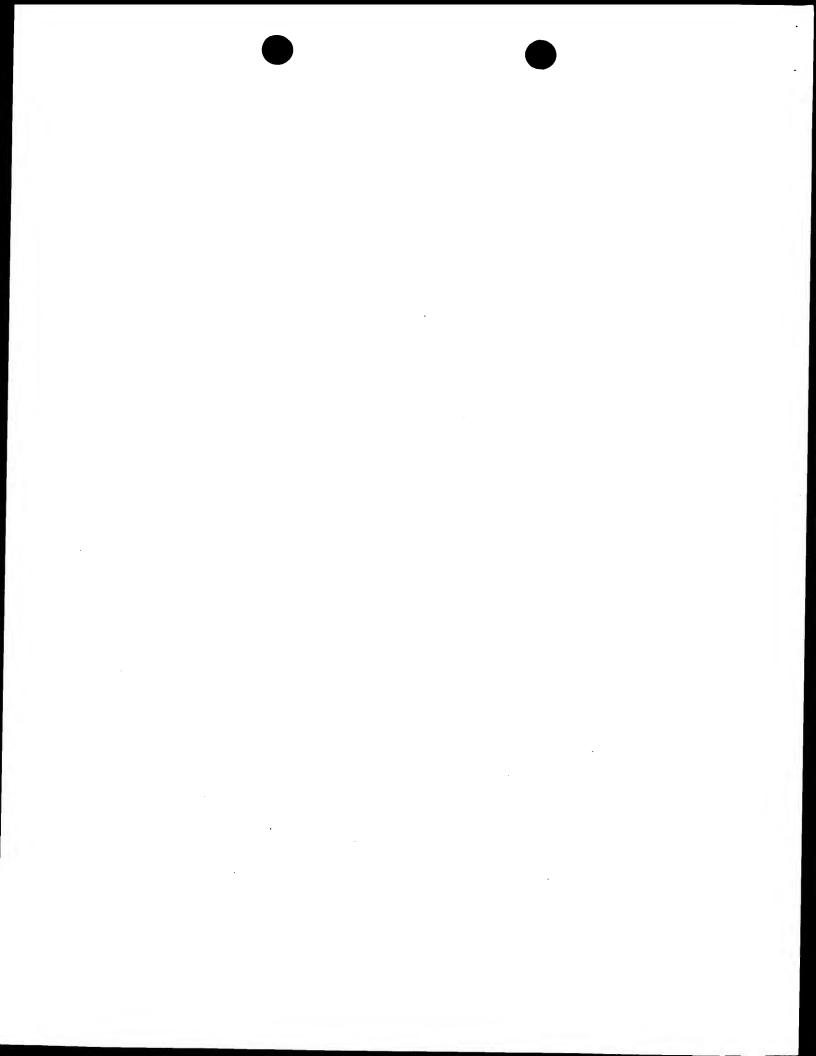
PCT/GB97/02838

7. An enzyme having significant (as herein defined) sequence similarity to IPNS, wherein at least one of the following amino acid residues is modified:

V272; L231; L223; P283; T221; F211; F285; Q330;

- 5 I187; V185; Y189; R279; S281; N230; Q225; N252; S210.
 - 8. A gene which codes for the enzyme of claim 6 or claim 7.
 - 9. A micro-organism containing the gene of claim 8 and which is capable of expressing the gene under fermentation conditions.
 - 10. Use of the micro-organism of claim 9 for making a bicyclic β-lactam of the penicillin or cephalosporin (including cephams) families.
 - 11. Use of the enzyme of claim 6 or claim 7 for the preparation *in* vitro of a bicyclic β -lactam of the penicillin and cephalosporin families.
 - 12. In a method for the preparation of an enzyme, selected from IPNS, DAOCS, DACS, DAOC/DACS and sequence-related enzymes, in crystalline form for X-ray diffraction studies, the improvement which consists in maintaining the enzyme under anaerobic conditions with dioxygen substantially absent.
 - 13. A method which comprises using the three dimensional structure of a first enzyme selected from IPNS, DAOCS, DACS,
- DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, for determining or predicting the structure of a second enzyme which is structurally related to the first enzyme but is not active in the penicillin or cephalosporin biosynthesis pathway, and using the structural information so obtained for modifying the second enzyme or for designing an inhibitor for the second enzyme.
 - 14. Use of the enzyme of claim 6 or claim 7 to convert a dipeptide to a 6- aminopenicillin or other bicyclic β -lactam.
 - 15. Use as claimed in claim 14, wherein the dipeptide has been produced by use of a peptide synthetase enzyme such as ACV synthetase optionally modified to optimise dipeptide production.

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(57) Abstract

A three-dimensional structure is described of a complex of isopenicillin N synthase (IPNS) with Fe and its substrate ACV. This structure is used to design modified enzymes IPNS, DAOCS, DACS, DAOC/DACS and other related enzymes of the penicillin and cephalosporin biosynthesis pathway, which modified enzymes may accept unnatural substrates or improve production efficiency or produce improved products. Specific modifications of specific amino acid residues are proposed and exemplified.

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CI	Côte d'Ivoire	KP	Democratic People's	NZ	New Zealand		
CM	Cameroon		Republic of Korea	PL	Poland		
CN	China	KR	Republic of Korea	PГ	Portugal		
CU	Cuba	KZ	Kazakstan	RO	Romania		
CZ	Czech Republic	LC	Saint Lucia	RU	Russian Federation		
DE	Germany	LI	Liechtenstein	SD	Sudan		
DK	Denmark	ŁK	Sri Lanka	SE	Sweden		
EE	Estonia	LR	Liberia	SG	Singapore		

INTERNATIONAL SEARCH REPORT

inal Application No PCT/GB 97/02838

A. CLASSIFICATION OF SUBJECT MATTER IPC 6 C12N15/52 C12 C12N9/00 C12P35/00 C12N1/21 According to International Patent Classification (IPC) or to both national classification and IPC **B. FIELDS SEARCHED** Minimum documentation searched (classification system followed by classification symbols) IPC 6 C12N Documentation searched other than minimum documentation to the extent that such documents are included in the fields searched Electronic data base consulted during the international search (name of data base and, where practical, search terms used) C. DOCUMENTS CONSIDERED TO BE RELEVANT Category ° Citation of document, with indication, where appropriate, of the relevant passages Relevant to claim No. Χ ROACH PL ET AL: "Crystal structure of 1 isopenicillin N synthase is the first from a new structural family of enzymes. NATURE 375 (6533) P700-4 JUN 22 1995, XP002059796 cited in the application see abstract; figures 1-3; table 1 X SCOTT RA ET AL: "X-ray absorption 1,2 spectroscopic studies of the high-spin iron(II) active site of isopenicillin N synthase: evidence for Fe-S interaction in the enzyme-substrate complex." BIOCHEMISTRY 31 (19) P4596-601 MAY 19 1992, XP002067783 see the whole document -/--Х Further documents are listed in the continuation of box C. Х Patent family members are listed in annex. Special categories of cited documents: *T* later document published after the international filing date "A" document defining the general state of the art which is not considered to be of particular relevance or priority date and not in conflict with the application but cited to understand the principle or theory underlying the invention "E" earlier document but published on or after the international "X" document of particular relevance; the claimed invention filing date cannot be considered novel or cannot be considered to involve an inventive step when the document is taken alone "L" document which may throw doubts on priority claim(s) or which is cited to establish the publication date of another "Y" document of particular relevance; the claimed invention citation or other special reason (as specified) cannot be considered to involve an inventive step when the "O" document referring to an oral disclosure, use, exhibition or document is combined with one or more other such docuother means ments, such combination being obvious to a person skilled document published prior to the international filing date but later than the priority date claimed *&* document member of the same patent family Date of the actual completion of the international search Date of mailing of the international search report 3 0, 06, 98 11 June 1998 Name and mailing address of the ISA Authorized officer European Patent Office, P.B. 5818 Patentlaan 2 NL - 2280 HV Rijswijk Tel. (+31-70) 340-2040, Tx. 31 651 epo nl, Gurdjian, D

Fax: (+31-70) 340-3016

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C.(Continu	ation) DOCUMENTS CONSIDERED TO BE RELEVANT	
Category °	Citation of document, with indication, where appropriate, of the relevant passages	Relevant to claim No.
X	ORVILLE, ALLEN M. ET AL: "Thiolate ligation of the active site iron(II) of isopenicillin N synthase derives from substrate rather than endogenous cysteine: spectroscopic studies of site-specific Cys.fwdarw. Ser mutated enzymes" BIOCHEMISTRY (1992), 31(19), 4602-12 CODEN: BICHAW;ISSN: 0006-2960, XP002067784 see the whole document	1,2
X	BLACKBURN JM ET AL: "A heuristic approach to the analysis of enzymic catalysis: reaction of delta-(L-alpha-aminoadipoyl)-L-cysteinyl-D-alpha-aminobutyrate and delta-(L-alpha-aminoadipoyl)-L-cysteinyl-D-allylglycine catalyzed by isopenicillin N synthase isozymes." BIOCHEMISTRY, JUN 6 1995, 34 (22) P7548-62, UNITED STATES, XP002067785 see the whole document	1,2
X	HUFFMAN GW ET AL: "Substrate specificity of isopenicillin N synthase." J MED CHEM, MAY 15 1992, 35 (10) P1897-914, UNITED STATES, XP002067786 see the whole document	1,2
A	DATABASE BIOTECHNOLOGY ABSTRACTS DERWENT ,LONDON aN 88-01715, PRATT A J: "Manipulation of beta-lactam biosynthetic enzymes" XP002067788 see abstract & ABSTR.PAP.AM.CHEM.SOC., 1987,	6-11,14, 15
Α	EP 0 307 171 A (LILLY CO ELI) 15 March 1989 see claims 1-8	1,2, 6-11,14, 15
A	EP 0 317 096 A (LILLY CO ELI) 24 May 1989	1,2, 6-11,14, 15
	see claims 1-18	
	-/	
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		PCT/GB 97/02838
.(Continuatio	on) DOCUMENTS CONSIDERED TO BE RELEVANT	Relevant to claim No.
Category ° C	Citation of document, with indication, where appropriate, of the relevant passages	
	TAN, DOREEN S. H. ET AL: "Functional analysis of conserved histidine residues in Cephalosporium acremonium isopenicillin N synthase by site-directed mutagenesis" J. BIOL. CHEM. (1996), 271(2), 889-94 CODEN: JBCHA3;ISSN: 0021-9258, XP002060004 see abstract see page 889, right-hand column, paragraph 2; figures 1,4; tables 2,3 see page 893, left-hand column, paragraph 2	1,2, 6-11,14, 15
A	KRIAUCIUNAS A ET AL: "The functional role of cysteines in isopenicillin N synthase. Correlation of cysteine reactivities toward sulfhydryl reagents with kinetic properties of cysteine mutants." J BIOL CHEM, JUN 25 1991, 266 (18) P11779-88, UNITED STATES, XP002060005 see abstract see page 11780, left-hand column, paragraph 3 see page 11782, right-hand column, line 12 - line 17	1,2, 6-11,14, 15
Р,Х	SAMI, MALKIT ET AL: "Glutamine-330 is not essential for activity in isopenicillin N synthase from Aspergillus nidulans" FEBS LETT. (1997), 405(2), 191-194 CODEN: FEBLAL; ISSN: 0014-5793, XP002059797 see the whole document	1,6-11, 14,15
P,X	ROACH, PETER L. ET AL: "Structure of isopenicillin N synthase complexed with substrate and the mechanism of penicillin formation" NATURE (LONDON) (1997), 387(6635), 827-830 CODEN: NATUAS; ISSN: 0028-0836, XP002067787 see the whole document	1,2
P,X	WO 97 20053 A (GIST BROCADES BV ;UNIV OXFORD (GB); SUTHERLAND JOHN DAVID (GB); BO) 5 June 1997 see claims 1-9; figure 1	6-11,14,
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Box I Observations who	ere certain claims were found unsearchable (Continuation of item 1 of first sheet)
This International Search Repo	ort has not been established in respect of certain claims under Article 17(2)(a) for the following reasons:
	(=)(=) (or the following feasons:
	o subject matter not required to be searched by this Authority, namely:
	Authority, namely:
2. Claims Nos.:	
an extent that no mear	p parts of the International Application that do not comply with the prescribed requirements to such ningful International Search can be carried out, specifically:
	San Specifically;
Claims Nos.: because they are depe	endent claims and are not doubt.
, 3000	endent claims and are not drafted in accordance with the second and third sentences of Rule 6.4(a).
Box II Observations where	e unity of invention is lacking (Continuation of item 2 of first sheet)
memational Searching Auth	hority found multiple inventions in this international application, as follows:
	See additional .
	see additional sheet
As all required additional searchable claims.	d search fees were timely paid by the applicant, this International Search Report covers all
Sindbig Claims,	dearch Heport covers all
As all searchable claims	could be searched without offer in the
of any additional fee.	could be searched without effort justifying an additional fee, this Authority did not invite payment
X As only some of the requi	ired additional search fees were timely paid by the applicant, this International Search Report for which fees were paid, specifically claims Nos
	red additional search fees were timely paid by the applicant, this International Search Report for which fees were paid, specifically claims Nos.:
1 2 6-11 14 15	
	
	arch fees were timely poid but
No required additional sea	first mentioned in the attended by the applicant. Consequently, this International Search Bonne
No required additional sea restricted to the invention	arch fees were timely paid by the applicant. Consequently, this International Search Report is first mentioned in the claims; it is covered by claims Nos.:
No required additional sea restricted to the invention	first mentioned in the claims; it is covered by claims Nos.:
No required additional sea restricted to the invention	first mentioned in the claims; it is covered by claims Nos.:
·	first mentioned in the claims; it is covered by claims Nos.:
No required additional sea restricted to the invention	
·	The additional search fees were accompanied by the applicant's protest. No protest accompanied the payment of additional search fees.

INTERNATIONAL SEARCH REPORT

International Application No. PCT/GB 97 /02838

FURTHER INFORMATION CONTINUED FROM PCT/ISA/ 210

This International Searching Authority found multiple (groups of) inventions in this international application, as follows:

1. Claim: 1 partly

IPNS complexed with Mn

2. Claim: 2 and 1 partly

IPNS complexed with Fe and ist substrate or an analogue of its substrate

3. Claims: 3-5, 13

the use of the three dimensional structure of a member of the IPNS family of enzymes to modify another enzyme .

4. Claims: 6-11,14-15

Enzyme having significant sequence similarity to IPNS wherein at least one of the following amino acid residues is modified ,r87,y189,s183,y91,f285,q330,t331 v185,l106,c104,v217,l324,l317,i325,l321,s210,v272,l231,l223,p283,t221,f211,i187,v185,y189,r279,s281,n230,q225,n252,r287,r88, mutants of an enzyme having similarity to IPNS, gene encoding it, micro-organism containing the gene and their use in beta-lactam production.

5. Claim: 12

methods of preparation of an enzyme of the IPNS family in crystalline form consisting of maintaining the crystalline enzymes of the IPNS family under anaeorobic conditions .

information on patent family members

PCT/GB 97/02838

Patent document cited in search report		Publication date		atent family nember(s)	Publication date
EP 0307171	A	15-03-1989	US AU AU DK FI JP CN	4885252 A 614988 B 2191788 A 493788 A 884112 A 1098493 A 1034578 A	05-12-1989 19-09-1991 09-03-1989 24-04-1989 09-03-1989 17-04-1989 09-08-1989
EP 0317096	A	24-05-1989	US AU DK	4950603 A 2455188 A 606088 A	21-08-1990 25-05-1989 15-06-1989
WO 9720053	Α	05-06-1997	ÁU	1097297 A	19-06-1997